Methods in Irradiation Experiment Modelling

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The Abdus Salam International Centre for Theoretical Physics

Outline

- Why modelling
- Building a computational model
- Verification and validation of a computational model
- Monte Carlo calculations
- Nuclear data
- Summary

About myself

- 2009 Ph D in Nuclear engineering, Faculty of mathematics and physicis, University of Ljubljana
- 2010, 2012, postdoc at Culham Centre for fusion energy, JET
- 2014+ Head of the Reactor physics division at the Jozef Stefan Institute, Ljubljana, Slovenija
- Theoretical and experimental reactor physics related to practical applications in power and research reactors, in particular:
  - integral reactor experiments, criticality experiments and calculations
  - evaluation of critical and other reactor physics experiments
  - Monte Carlo transport of neutrons and photons in fission and fusion nuclear reactors

Why modelling

- Experiments
  - expensive (t & €) !
  - Difficult to perform with low uncertainty
  - Sometimes impossible to perform
- Calculations
  - Relatively cheap (t & €)
  - Relatively easy to perform
  - Practically everything can be calculated
  - Reliability, validity !!!

Neutron transport calculations

- deterministic codes
  - based on numerical or rarely analytical solving of neutron transport or diffusion equation
  - the computing errors are systematic
    - uncertainties in the cross section data
    - discretization of time-space-energy phase space
    - geometrical simplifications
  - computationally cheap ➔ PC
- Monte Carlo codes
  - capable of treating very complex three-dimensional configurations
  - continuous treatment of energy, as well as space and angle ➔ eliminates discretization errors
  - the computing errors are systematic and random
    - uncertainties in the cross section data (systematic)
    - other uncertainties (random)
  - computationally expensive ➔ need for large computer clusters

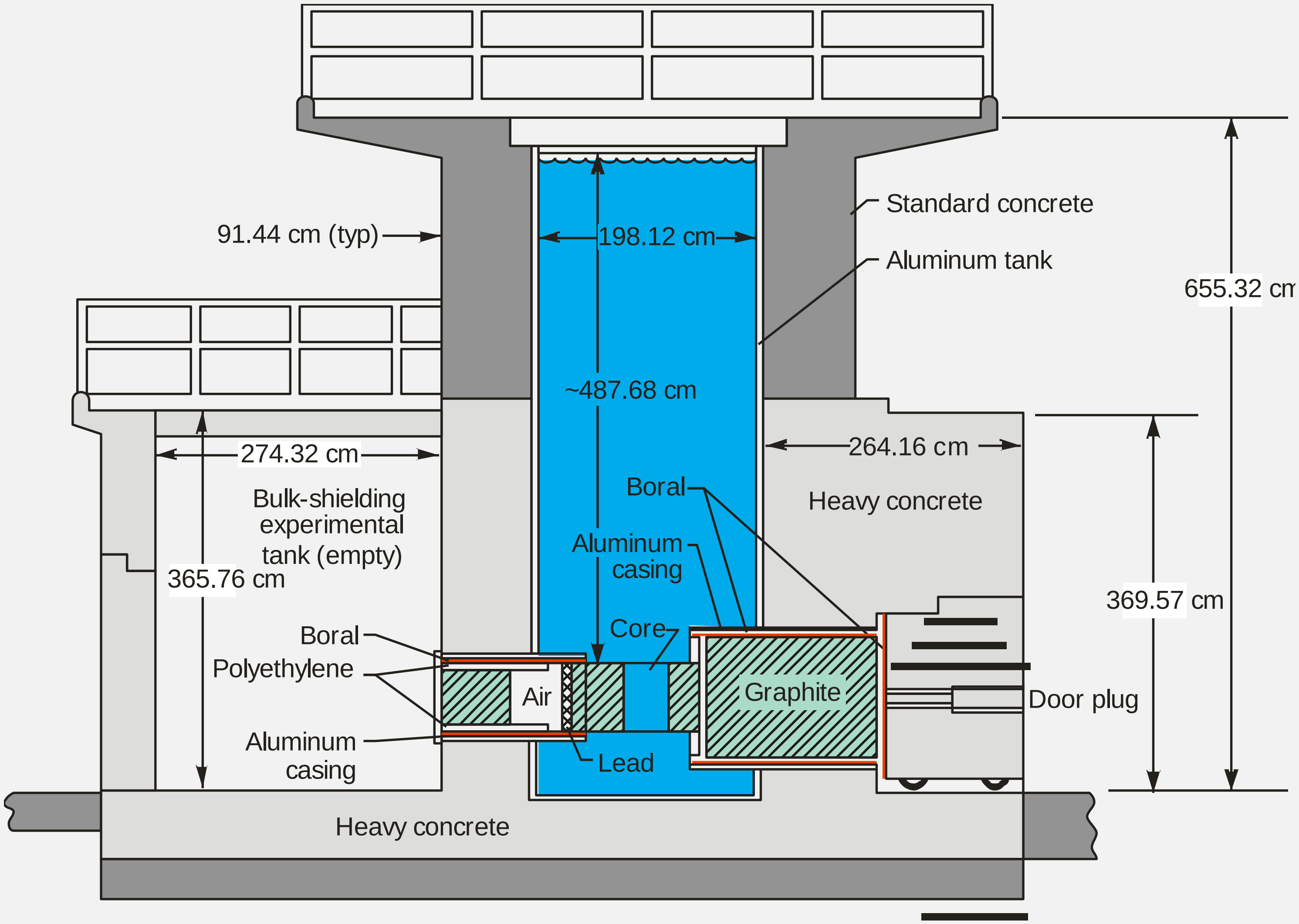
Building a reactor model

- first step is to collect
  - material
  - geometry
  - operational data of the reactor
- the task is not trivial if we try to collect *"**as built**" a*nd not just typical or generic data of particular reactor
- the set of data required for the calculation depends also on
  - the computer code
  - the problems which is solved
  - Diffusion codes require only general reactor geometry and dimensions
  - Monte Carlo codes require detailed geometry and materials

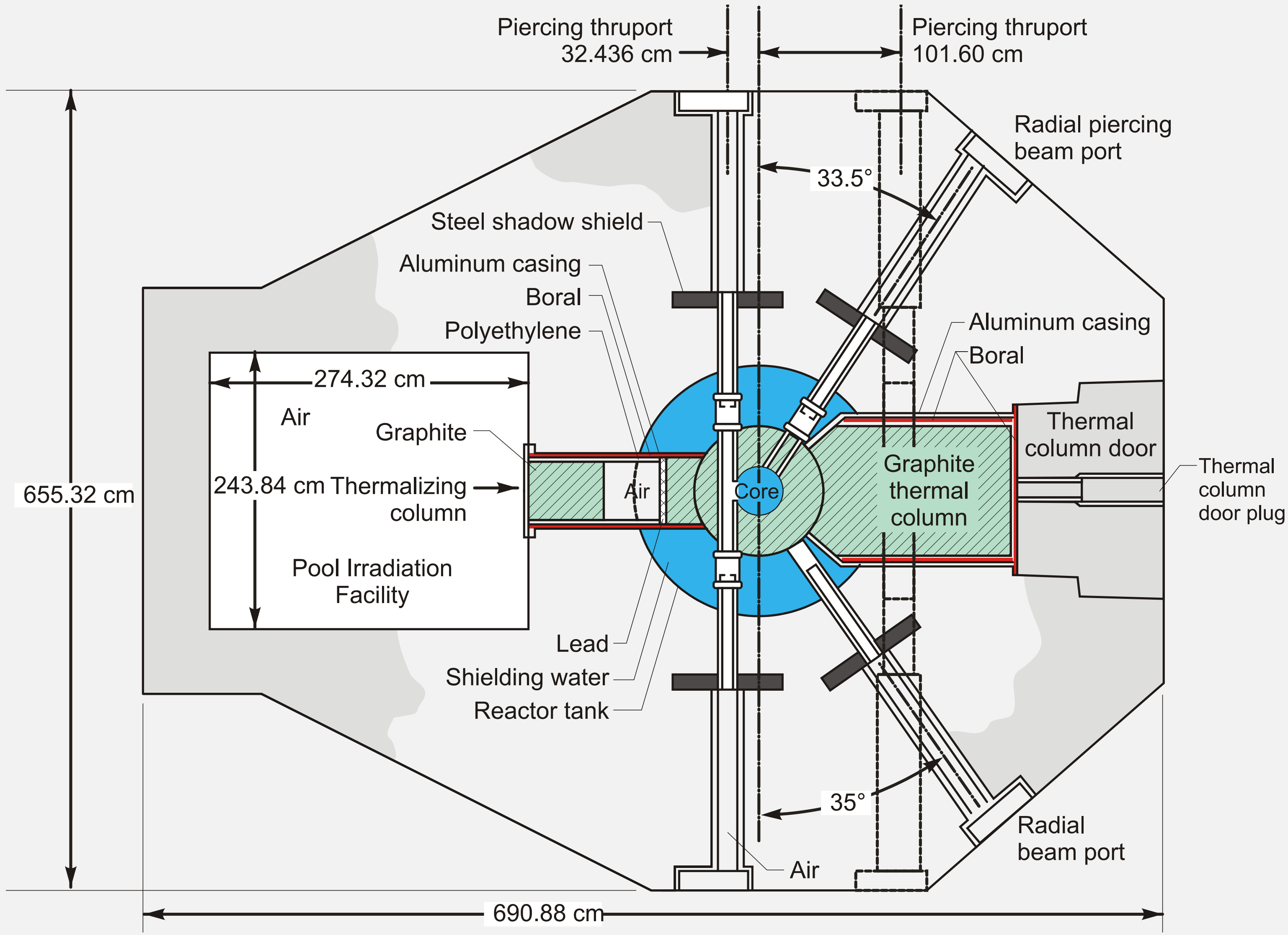
Building a model: an example

- JSI TRIGA

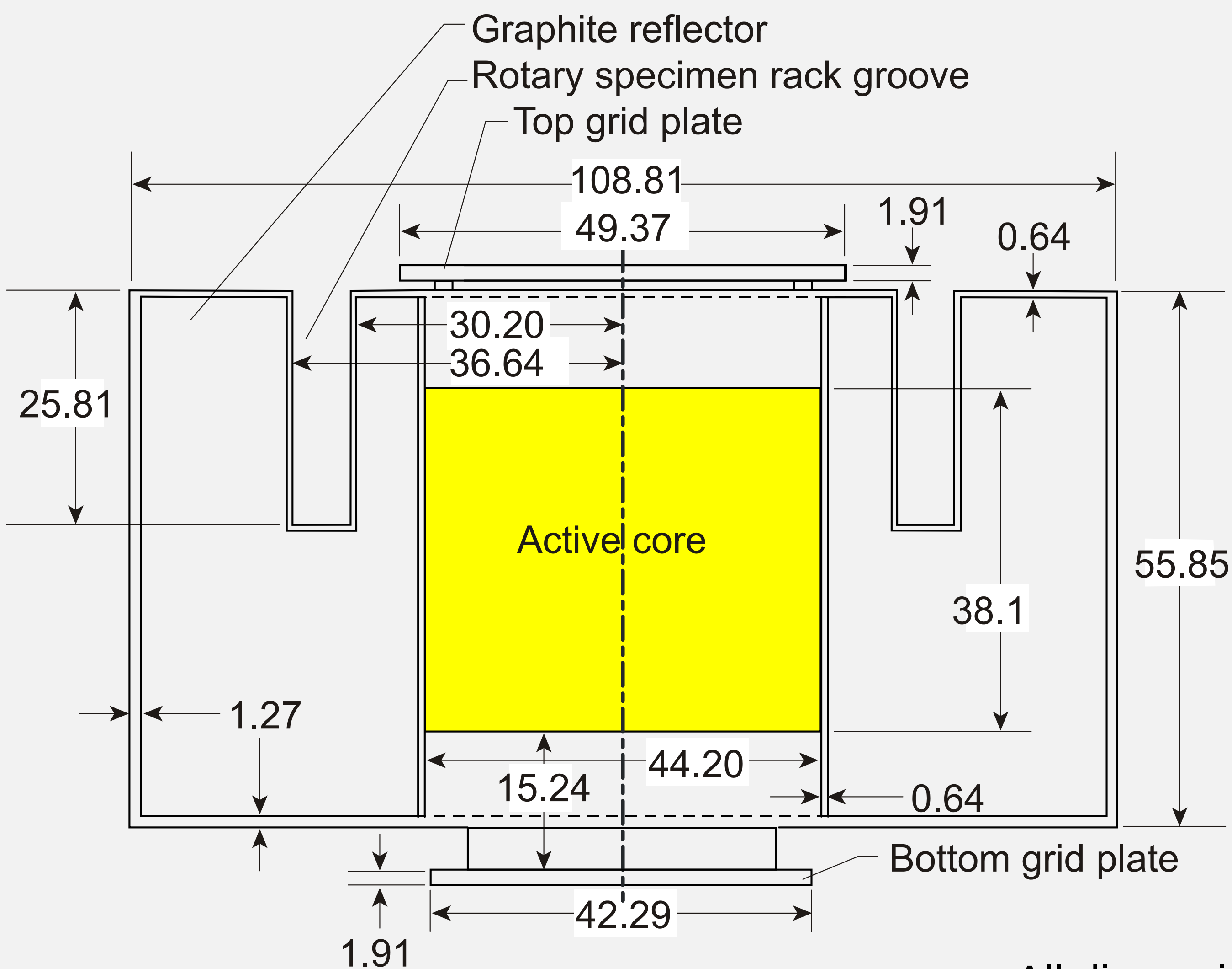
TRIGA Mark II: side view



TRIGA Mark II: top view



TRIGA Mark II: reflector

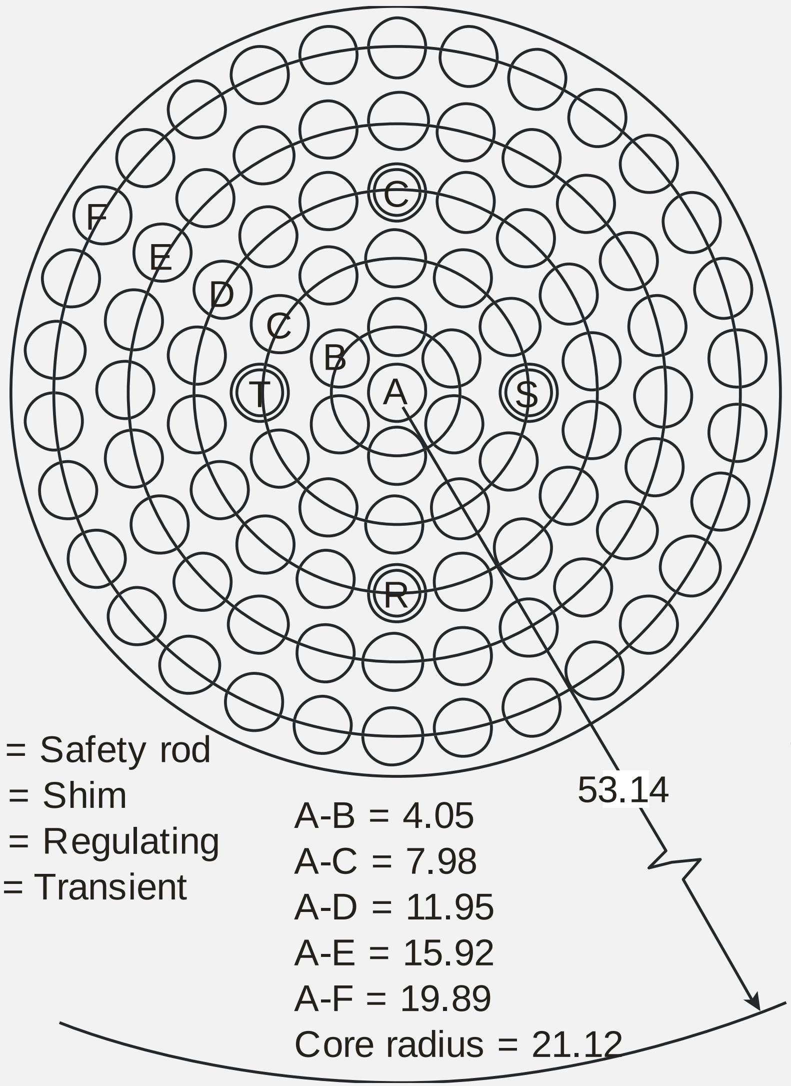


Dimensions in cm

All dimensions are in cm

C98 0953

TRIGA Mark II: core

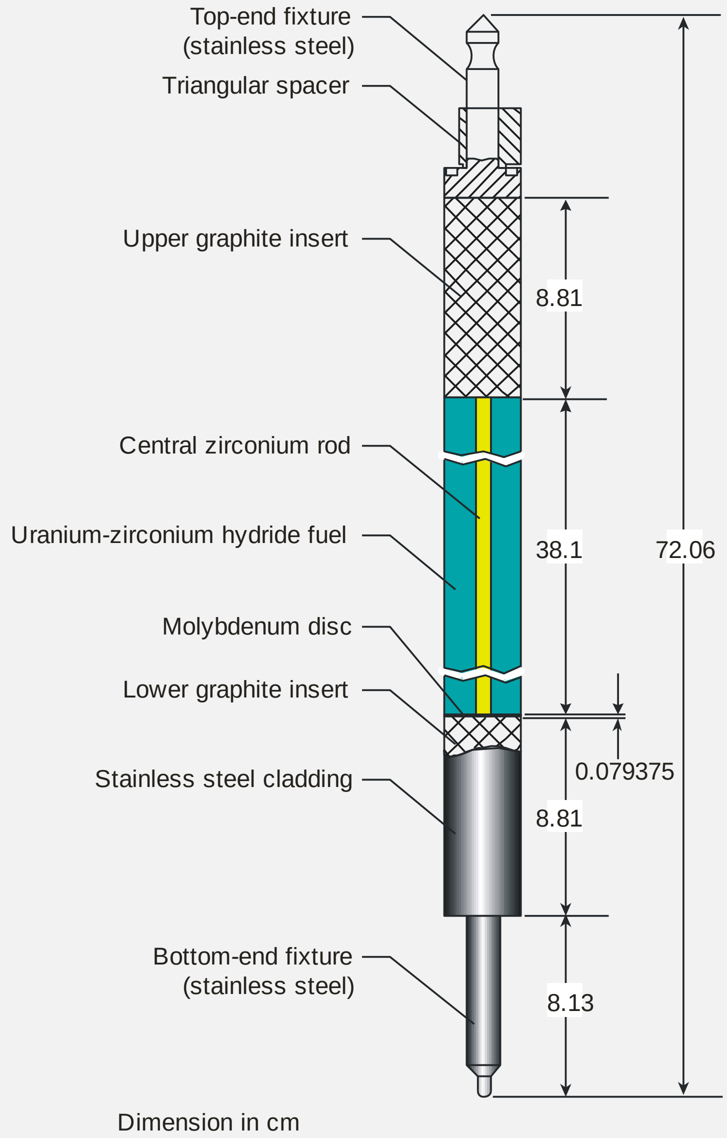


S = Safety rod
C = Shim
R = Regulating
T = Transient

A-B = 4.05
A-C = 7.98
A-D = 11.95
A-E = 15.92
A-F = 19.89
Core radius = 21.12

All dimensions are in cm

TRIGA Mark II: fuel element



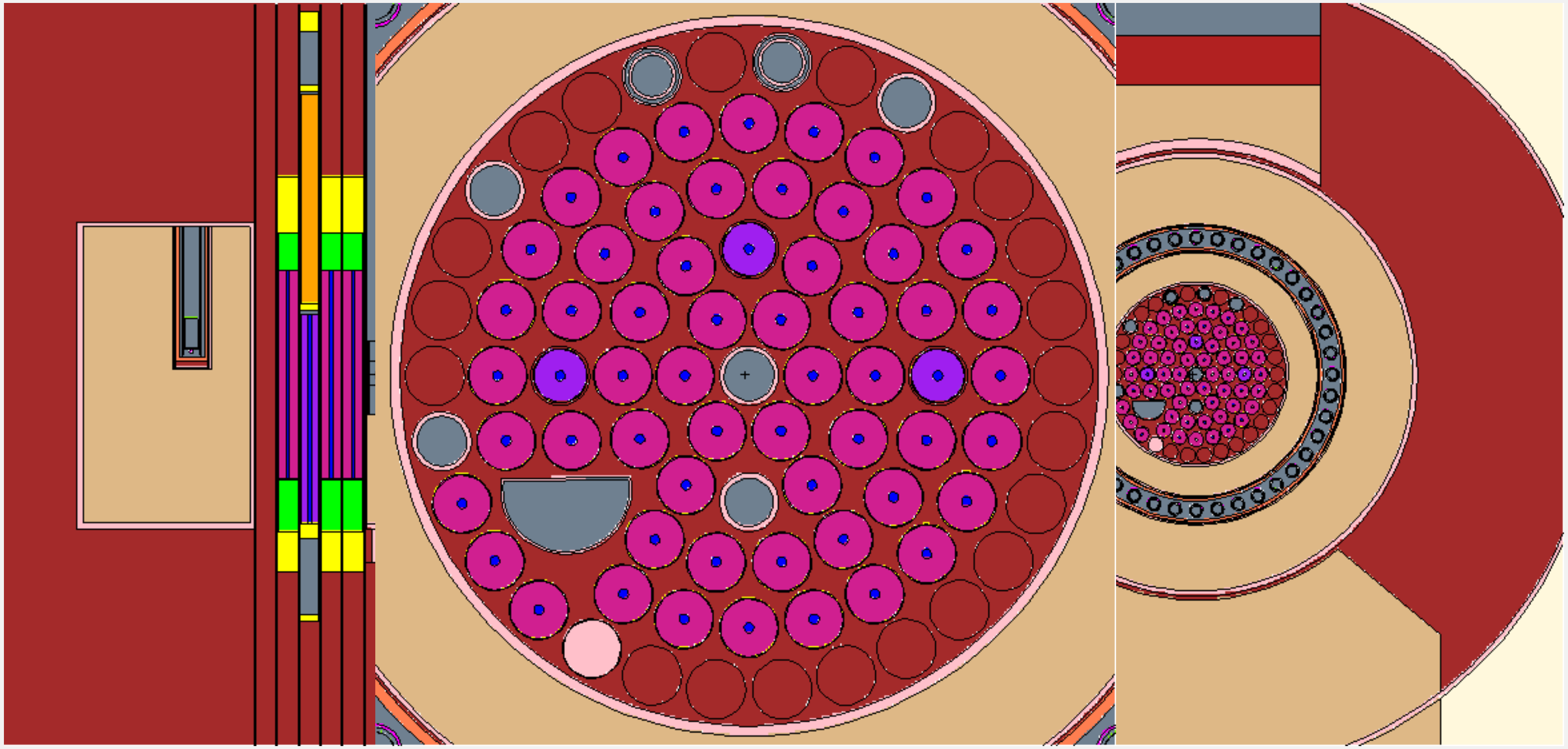
All dimensions are in cm

Triga: Fuel rod types

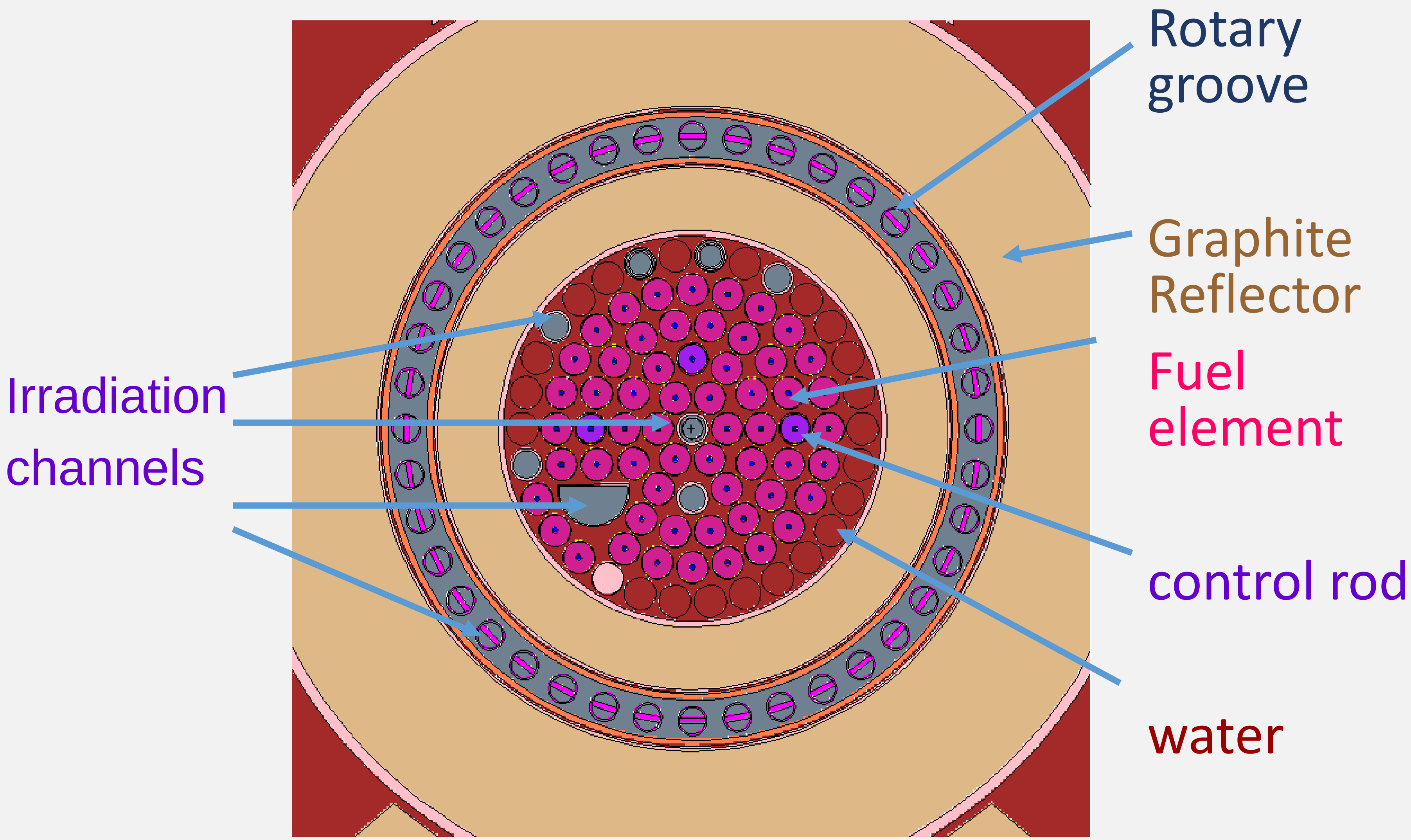
Physical characteristics				
	fuel		cladding	
material	$U\text{-}ZrH_x$		stainless steel	
inner diameter	0.635 cm		3.703 cm	
outer diameter	3.645 cm		3.754 cm	
length	38.10 cm		-	
Fuel material composition				
fuel rod (FR) name	8.5 FR	12 FR	20 FR	30 FR
U concentration [w/o]	8.5	12	20	30
$U\text{-}ZrH_x$ mass [g]	2235	2318	2462	2500
U enrichment	20	20	20	20
H:Zr	1.6	1.6	1.6	1.6
^{235}U mass [g]	38	55.6	99	150
Er concentration [w/o]	0	0	0.44	0.6

Computational model

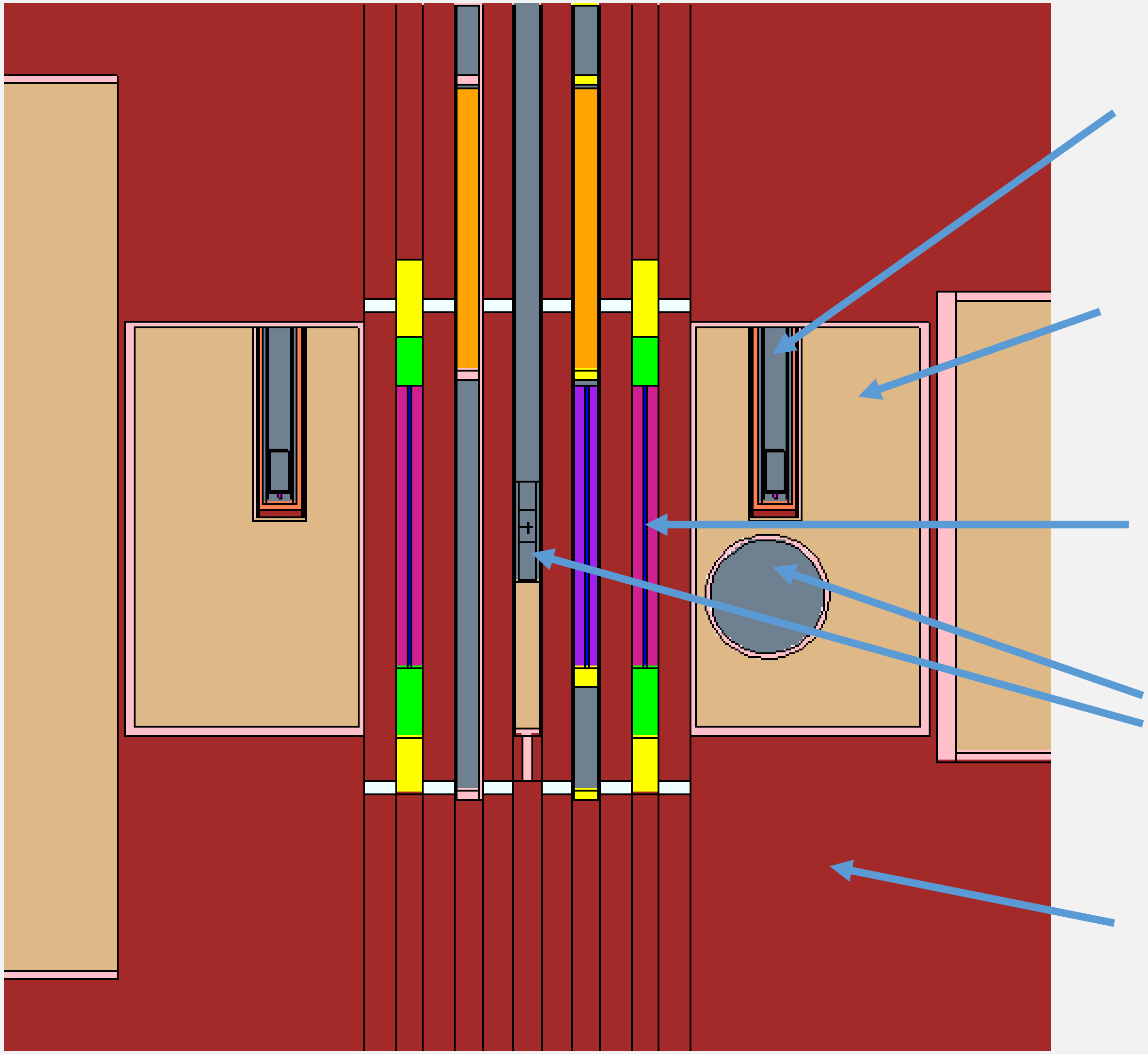
- room temperature (T = 20 °C)
- fresh fuel (BU = 0 MWd)
- continuous energy scale



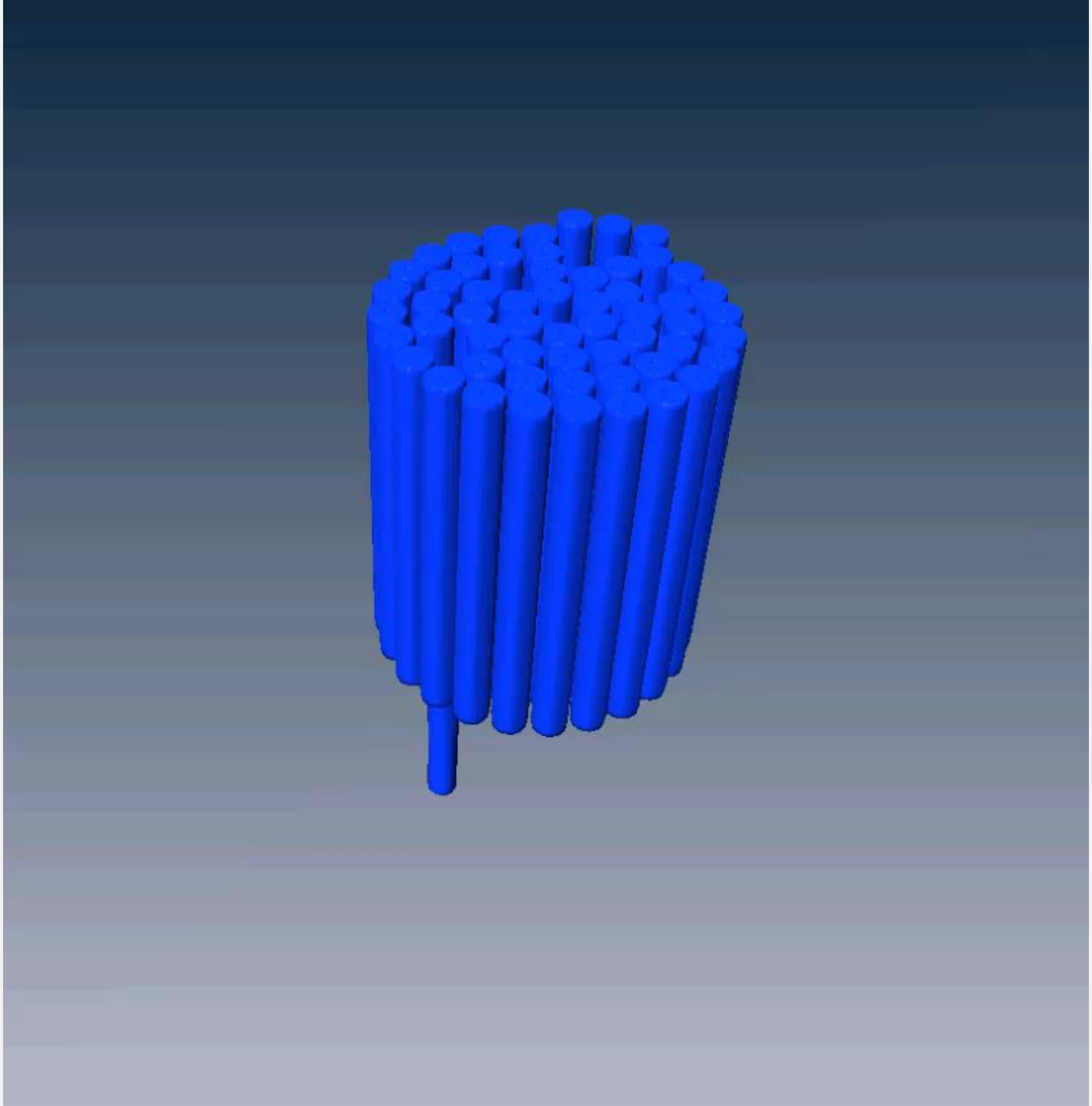
Computational model- top view



Computational model- side view



- Rotary groove
- Graphite Reflector
- Fuel element
- Irradiation channels
- water



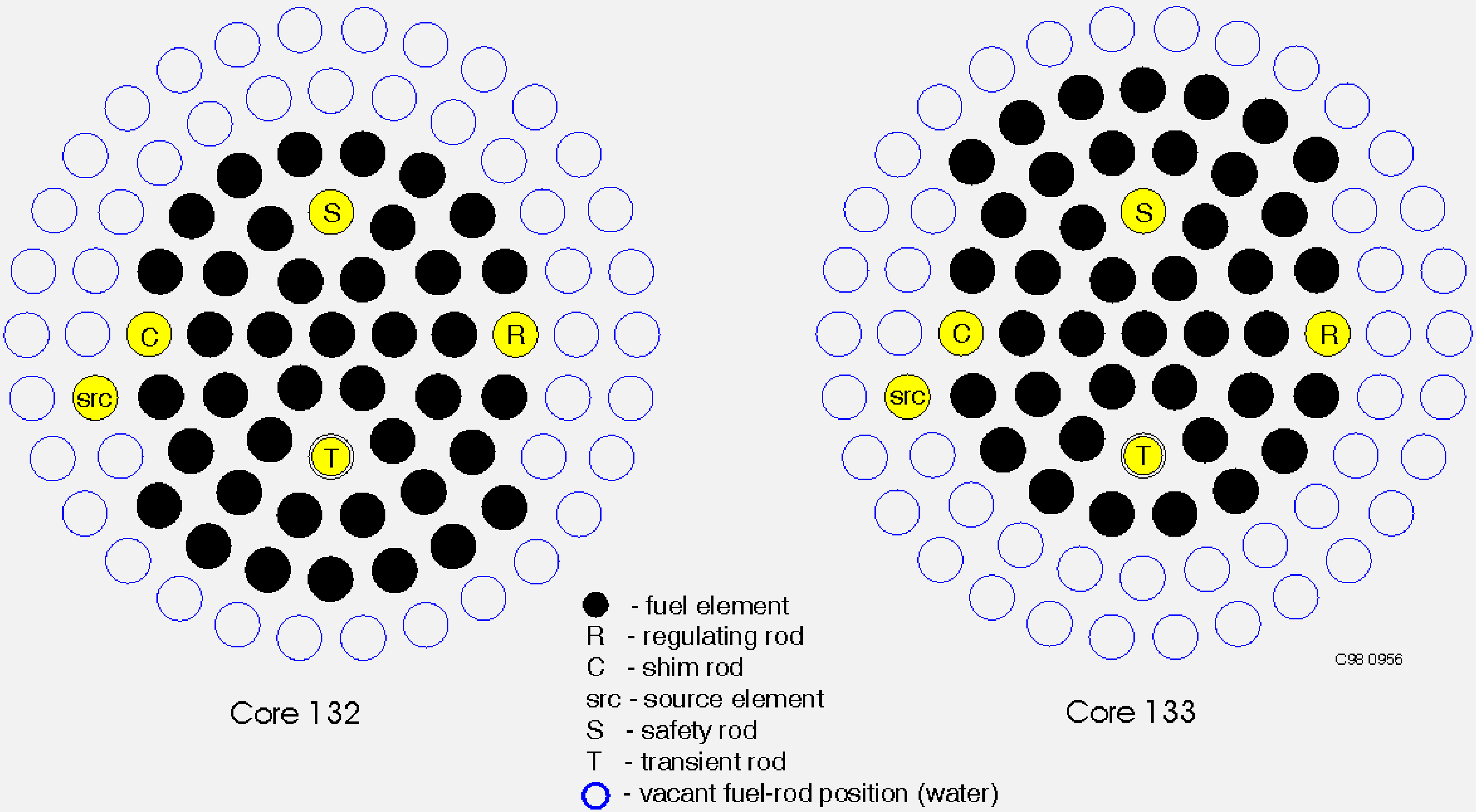
Verification and validation of the model

- the calculated result is valuable only if we know:
  - reliability
  - uncertainty
- user of any computer code should not only know how the code works but has to be familiar also with the **validity** and the **limitations** of the code
- VERIFICATION – check that the code does what is expected to do
- VALIDATION - one has to compare the calculated results with experiments to verify the results
- verification and validation (V&V) the most important part of reactor calculations

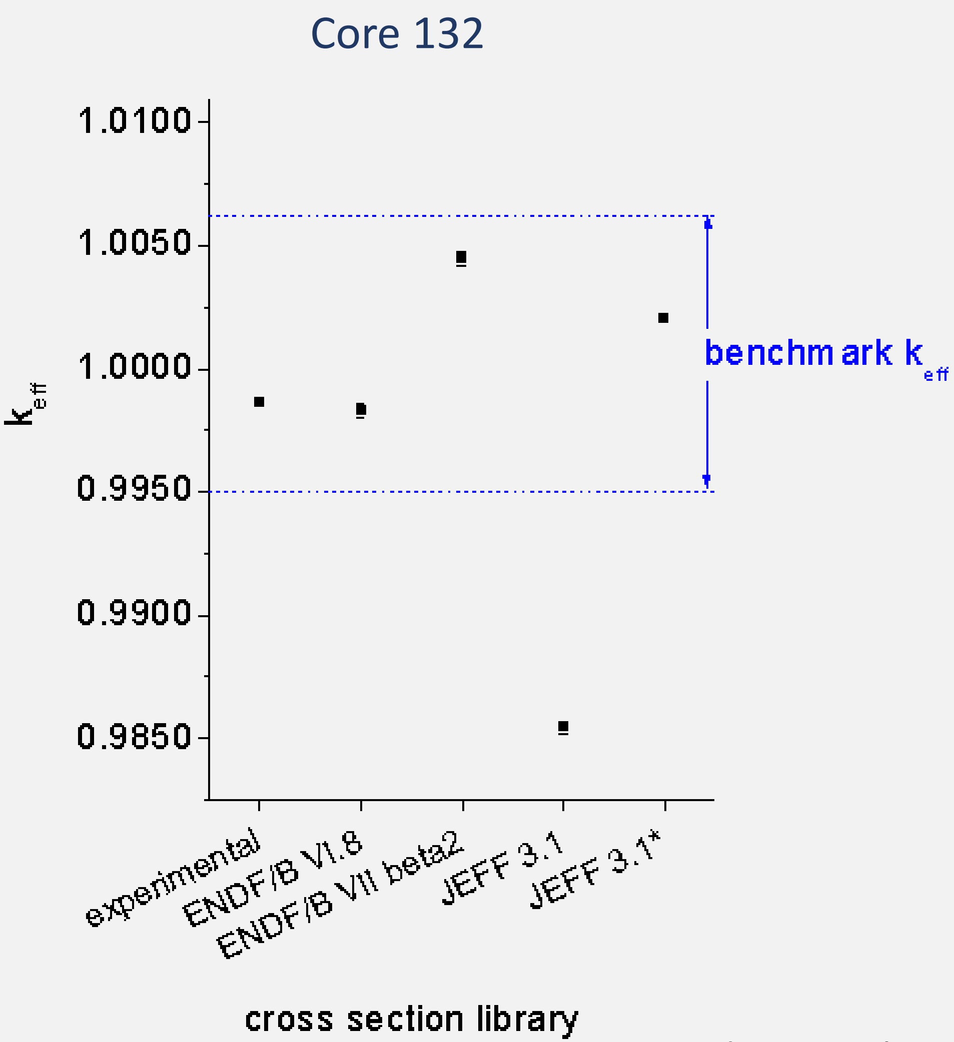
Approach

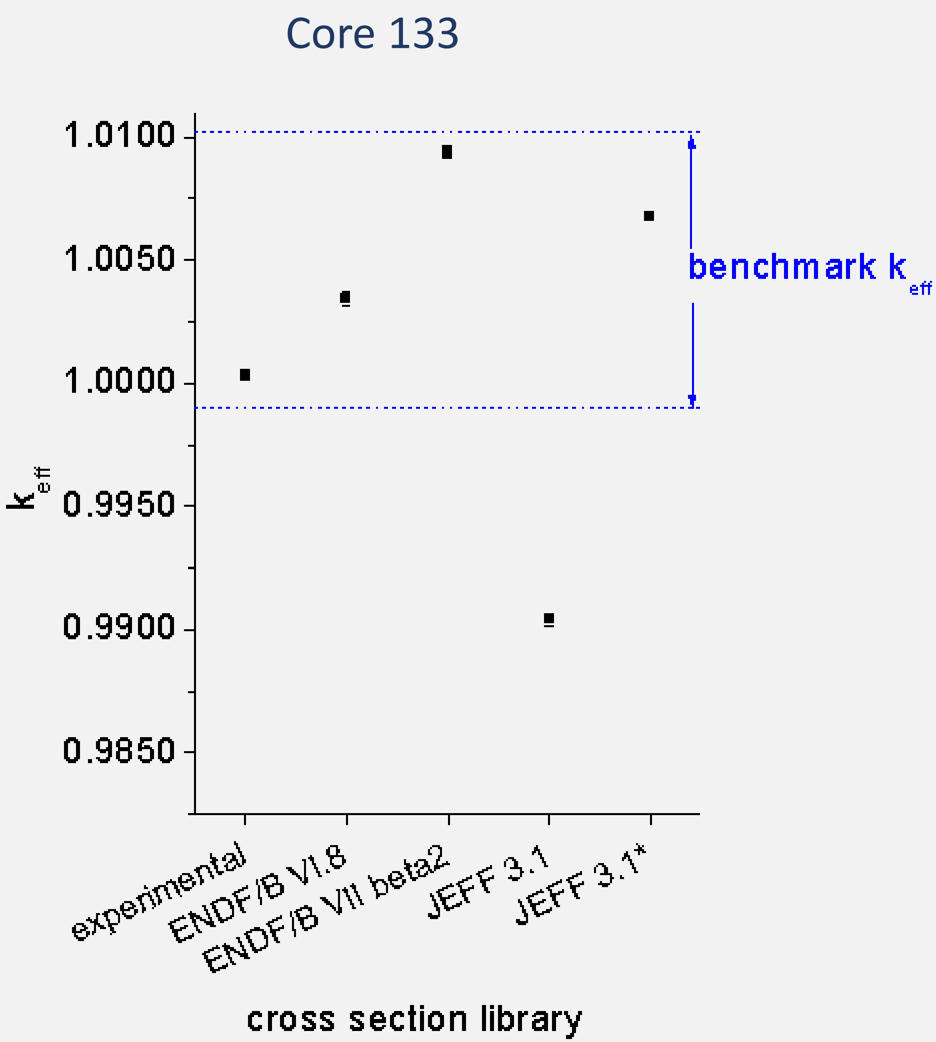
- Make a detailed computational model of the TRIGA reactor in MCNP (later TRIPOLI, SERPENT, OPENMC)
- Validate calculation by measurements
- Use the validated model for safety analyses and to support experimental campaigns
  - Absolute neutron flux
  - Neutron flux spectra
  - Dose rates
  - Gamma flux and dose

Criticality benchmark core



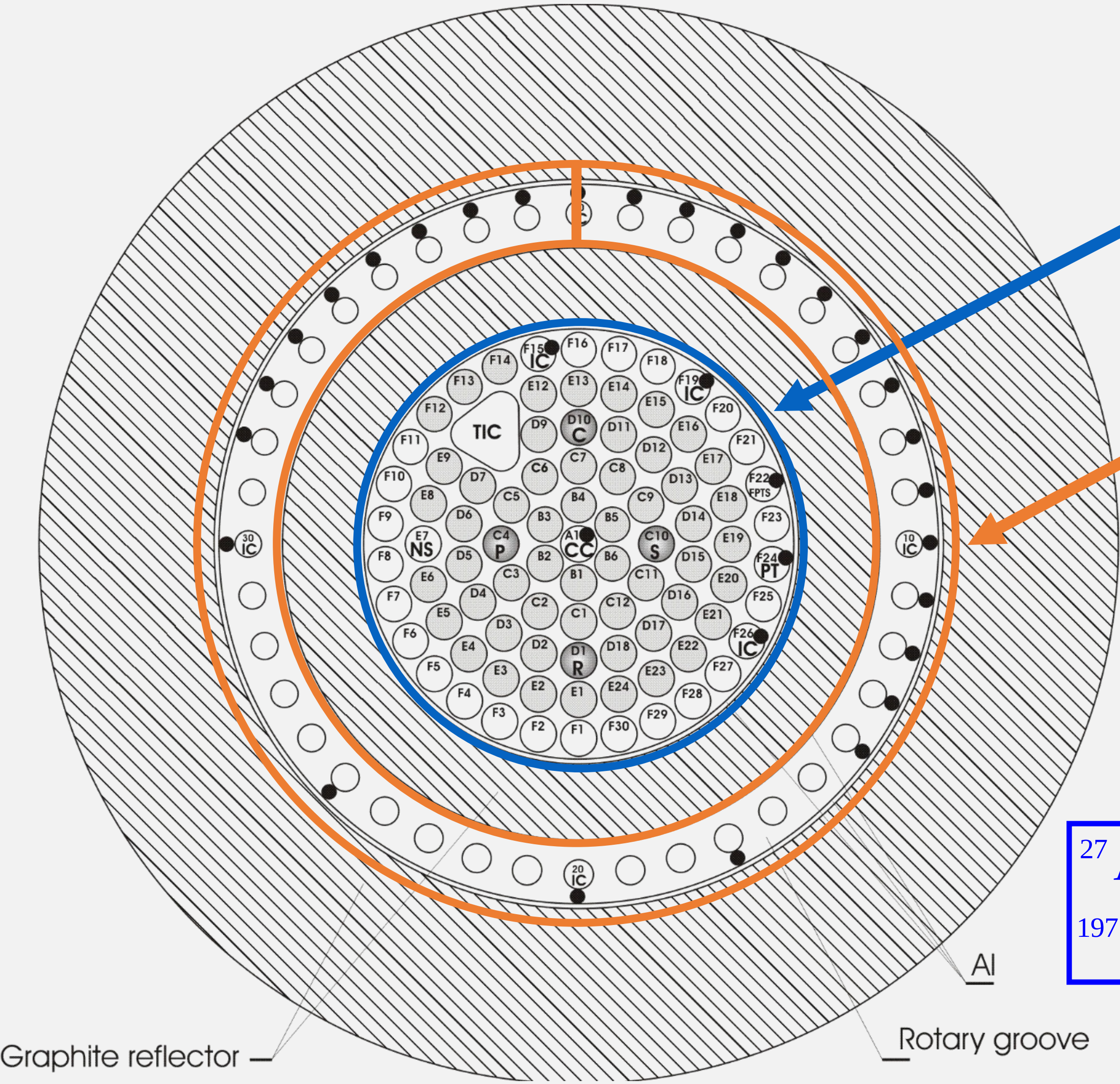
benchmark core k_{eff} comparison





* IAEA S(α,β)

Neutron flux distribution measurements



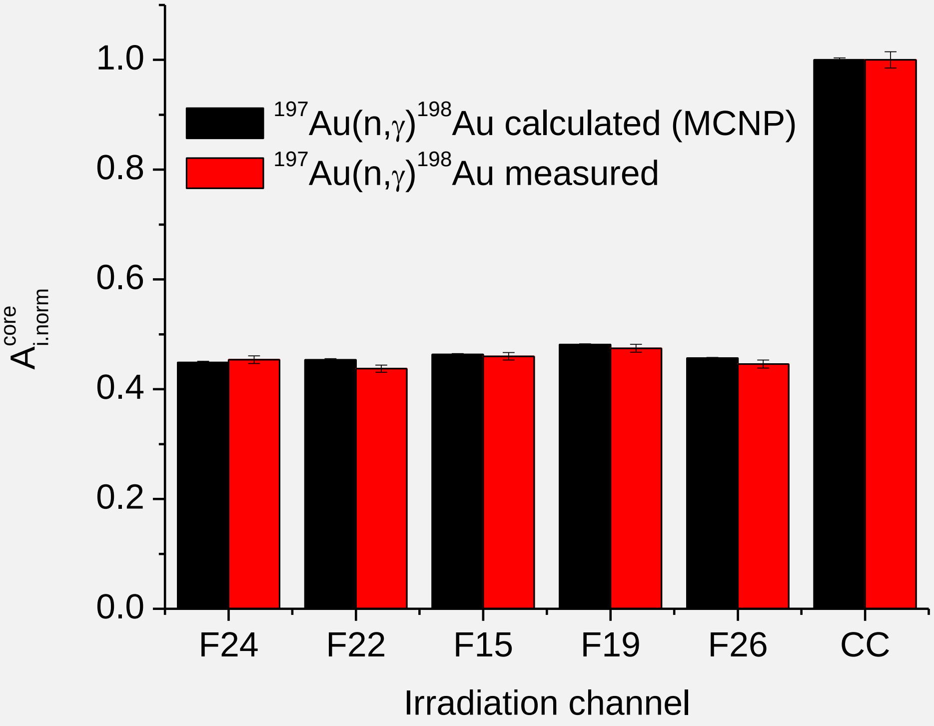
Foils: Al (99.9 w/o)-Au (0.1 w/o)

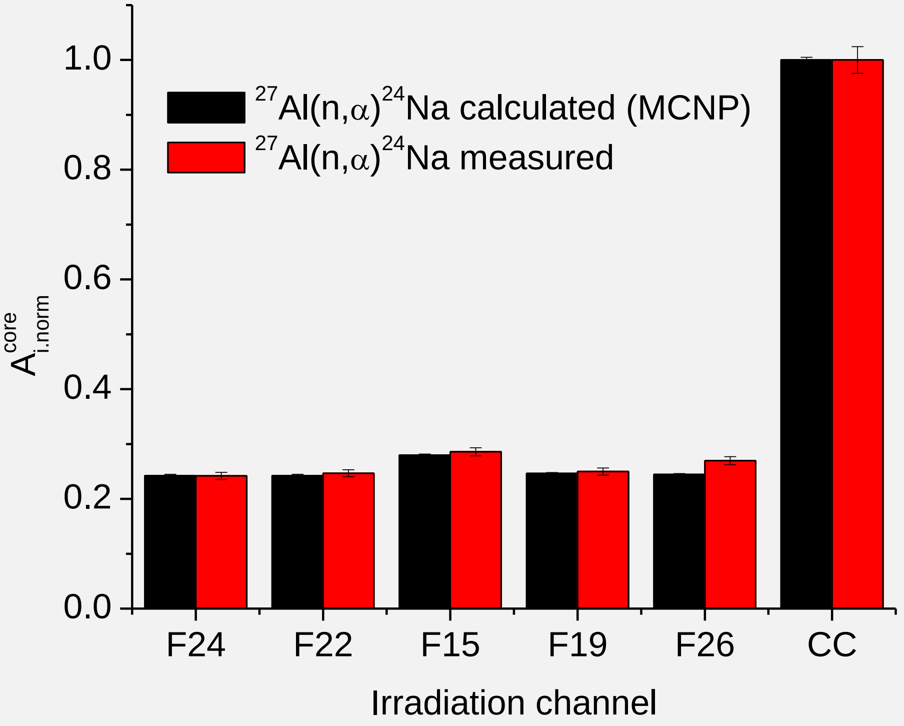
T_{irr} = 73 min at 250 kW

$$^{27}\text{Al}\,(n,\alpha)\ {}^{24}\text{Na}^{*} \xrightarrow{\gamma\,(E = 1368.6\ \text{keV})} {}^{24}\text{Na}$$

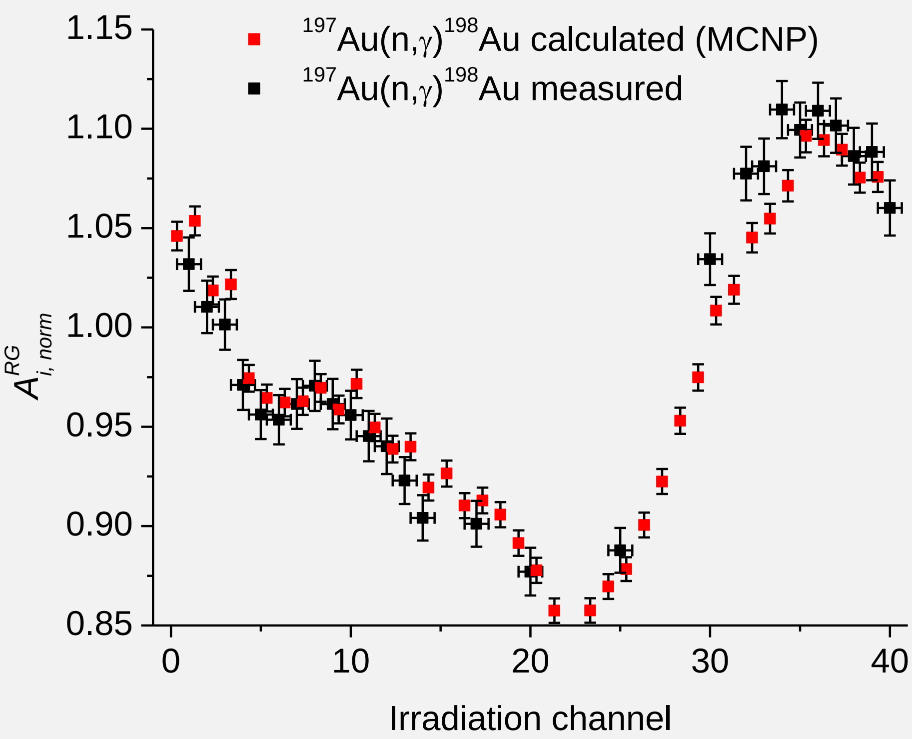
$$^{197}\text{Au}\,(n,\gamma)\ {}^{198}\text{Au}^{*} \xrightarrow{\gamma\,(E = 411.8\ \text{keV})} {}^{198}\text{Au}$$

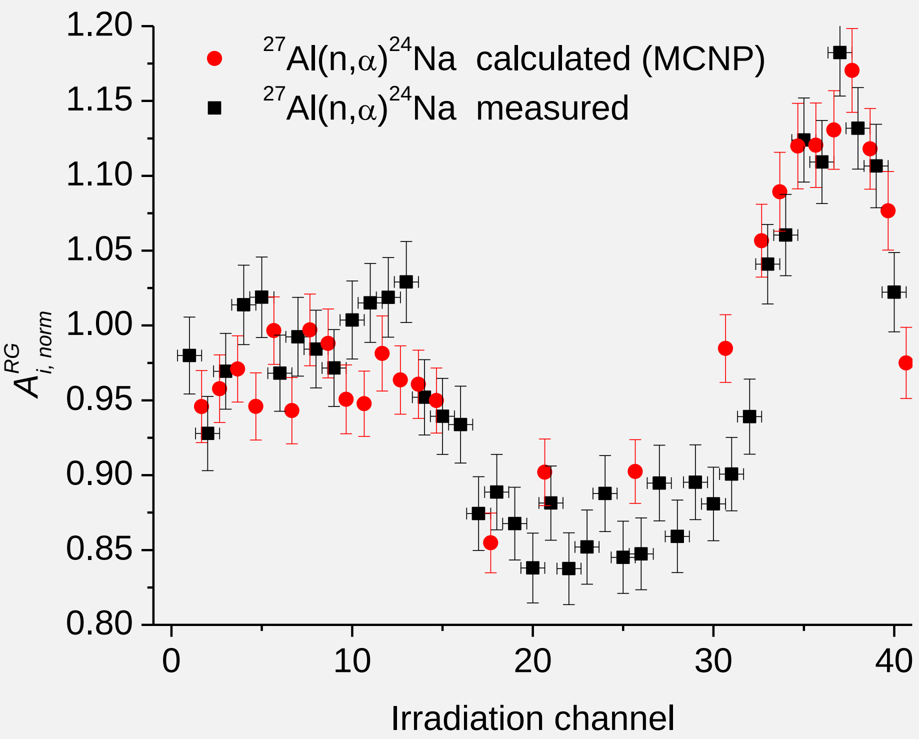
Results - core





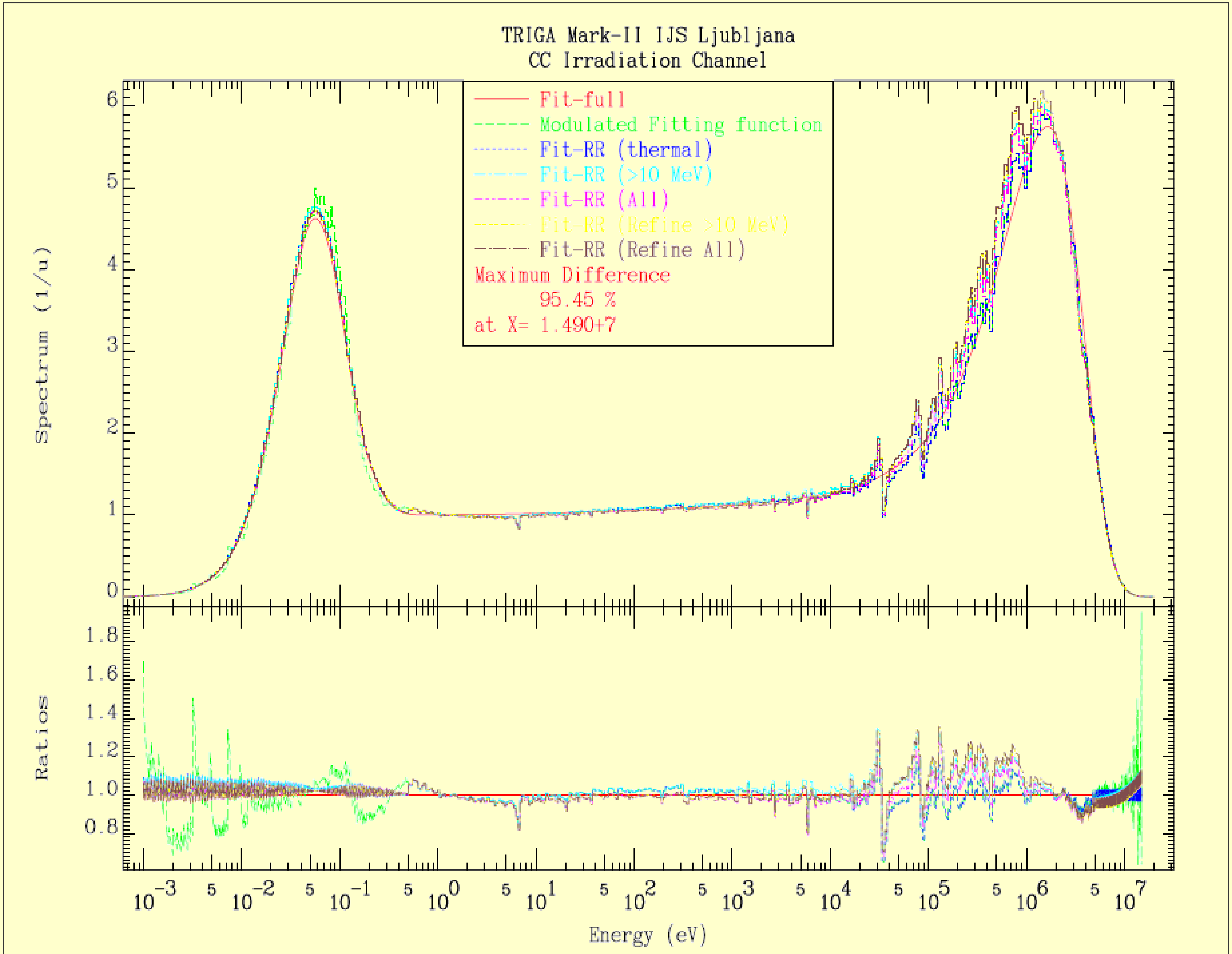
Results – carrousel facility



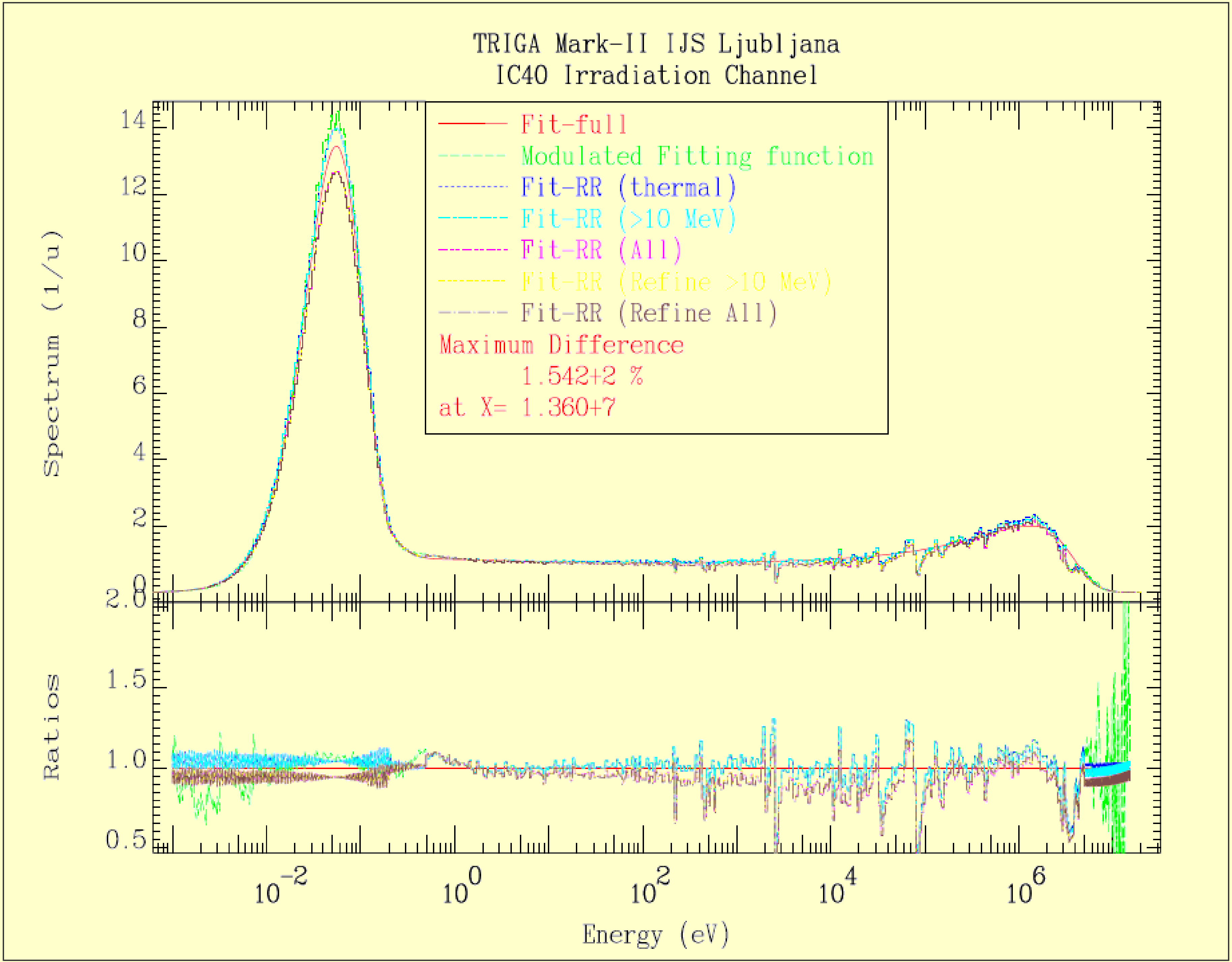


Neutron spectrum measurements

- 4 irradiation channels (1 core centre, 2 core periphery, 1 carrousel facility in the reflector)
- The neutron spectrum adjustments performed by the JSI-developed code GRUPINT based on the dosimetry library IRDFF
- monitors
  - Al (99.9 w/o)-Au (0.1 w/o)
  - Ni (80.93 w/o)- Mo (15.16 w/o)-W (2.76 w/o)- Mn (0.41 w/o)- Au(0.29 w/o)
  - Zr (99.8 w/o)
  - Zn (99.99 w/o)
- reactions
  - ^{27}Al(n,α), ^{27}Al(n, γ), ^{197}Au(n,γ)
  - ^{58}Ni(n,p), ^{92}Mo(n,p), ^{64}Ni(n,γ), ^{98}Mo(n,γ), ^{100}Mo(n,γ), ^{55}Mn(n,γ), ^{186}W(n,γ), ^{198}Au(n,γ)
  - ^{90}Zr(n,p), ^{90}Zr(n,2n), ^{94}Zr(n, γ), ^{96}Zr(n, γ)
  - ^{66}Zn(n,p), ^{64}Zn(n,γ), ^{68}Zn(n,γ), ^{70}Zn(n,γ)



TRIGA Mark-II IJS Ljubljana
CC Irradiation Channel
Fit-full
Modulated Fitting function
Fit-RR (thermal)
Fit-RR (>10 MeV)
Fit-RR (All)
Fit RR (Refine >10 MeV)
Fit-RR (Refine All)
Maximum Difference
95.45 %
at X= 1.490+7
Spectrum (1/u)
Ratios
Energy (eV)

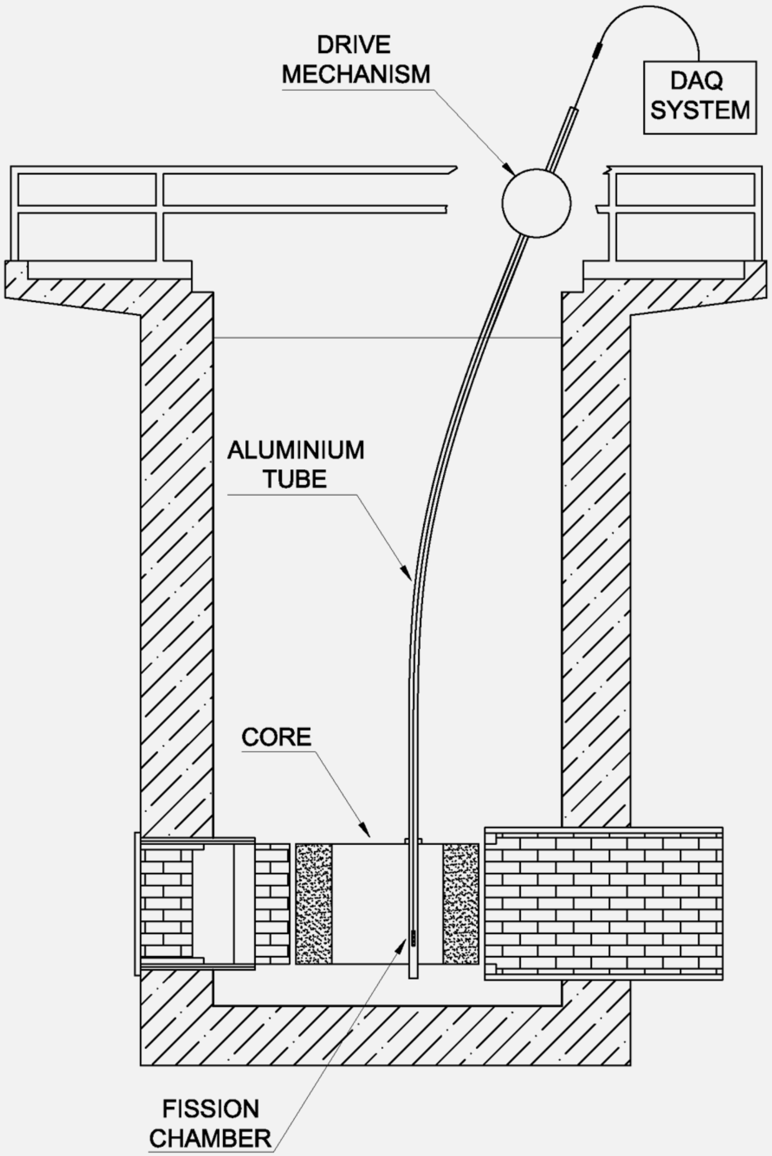


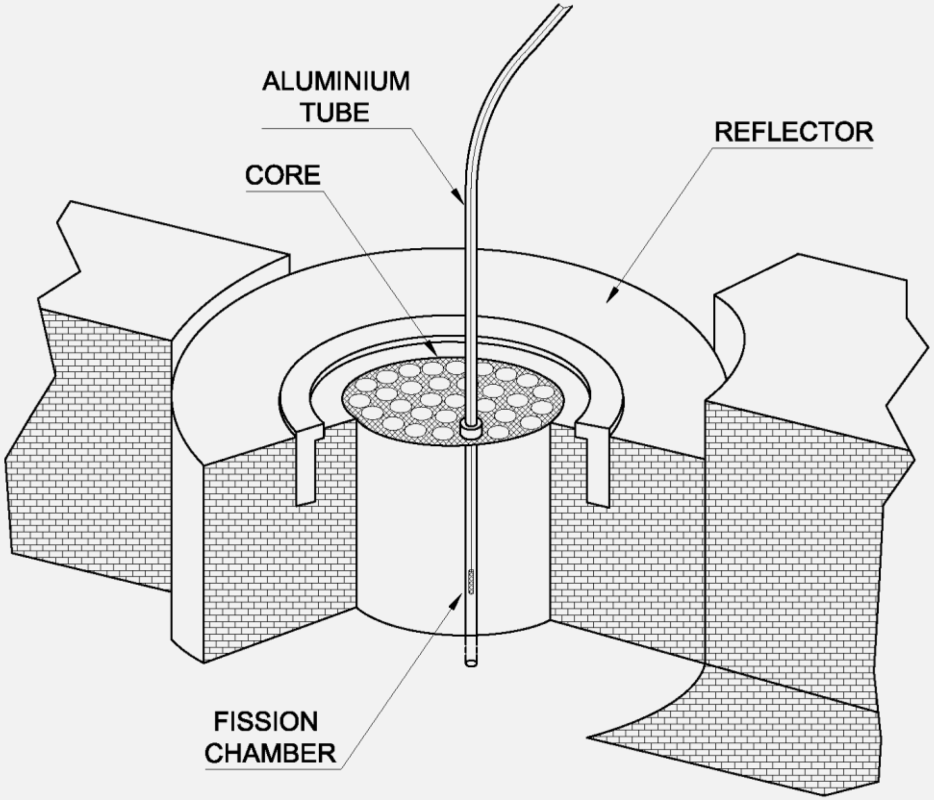
TRIGA Mark-II IJS Ljubljana
IC40 Irradiation Channel
Fit-full
Modulated Fitting function
Fit-RR (thermal)
Fit-RR (>10 MeV)
Fit-RR (All)
Fit-RR (Refine >10 MeV)
Fit-RR (Refine All)
Maximum Difference
1.542+2 %
at X= 1.360+7
Spectrum (1/u)
Ratios
Energy (eV)

Reaction rate profile measuremenmts

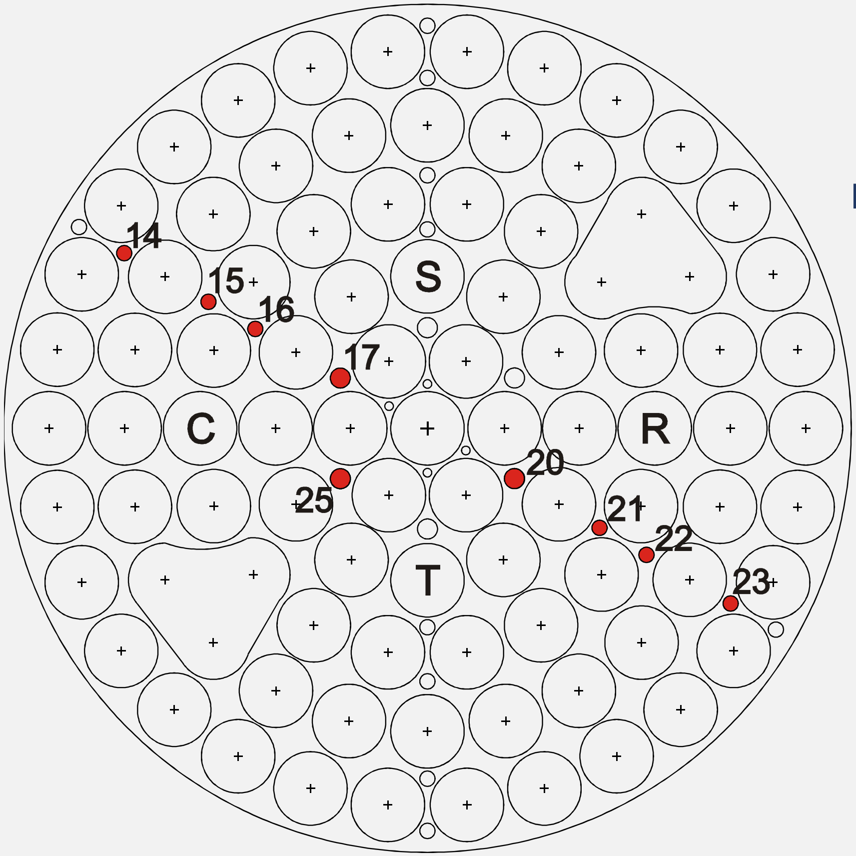
- Absolutely calibrated fission chamber (CEA)
  - 98.49 % enriched ^{235}U
  - Sensitive height ~4 mm
  - Diameter ~3 mm
- Au wires (JSI)
  - Al (99.9 w/o)-Au (0.1 w/o)
  - Activity measurements performed at JSI

Experimental setup 1





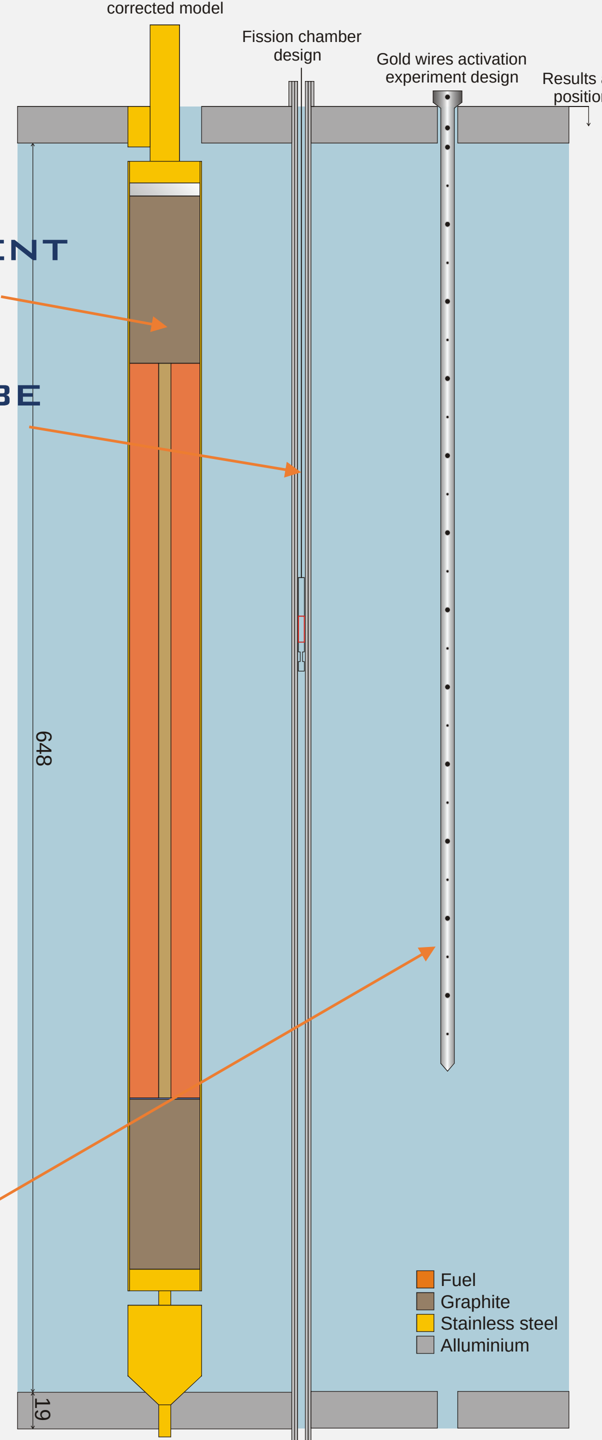
Experimental setup 2



FUEL ELEMENT

FC AL GUIDE TUBE

AL ROD FOR AU ACTIVATION MEASUREMENTS



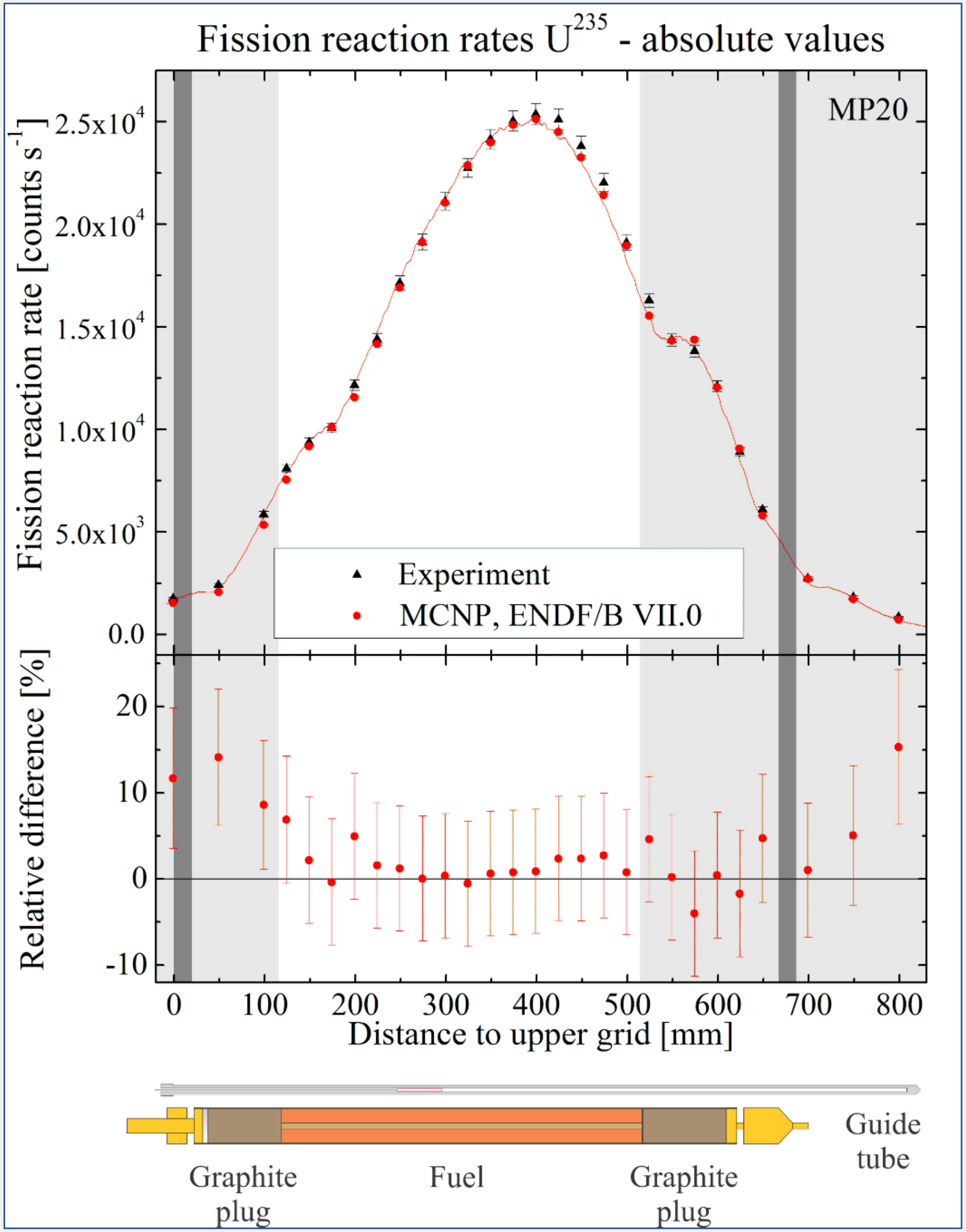
FISSION RATE AXIAL SCANS

Fission chamber

^{235}U (98.5 %)

Reactor power:

100 W



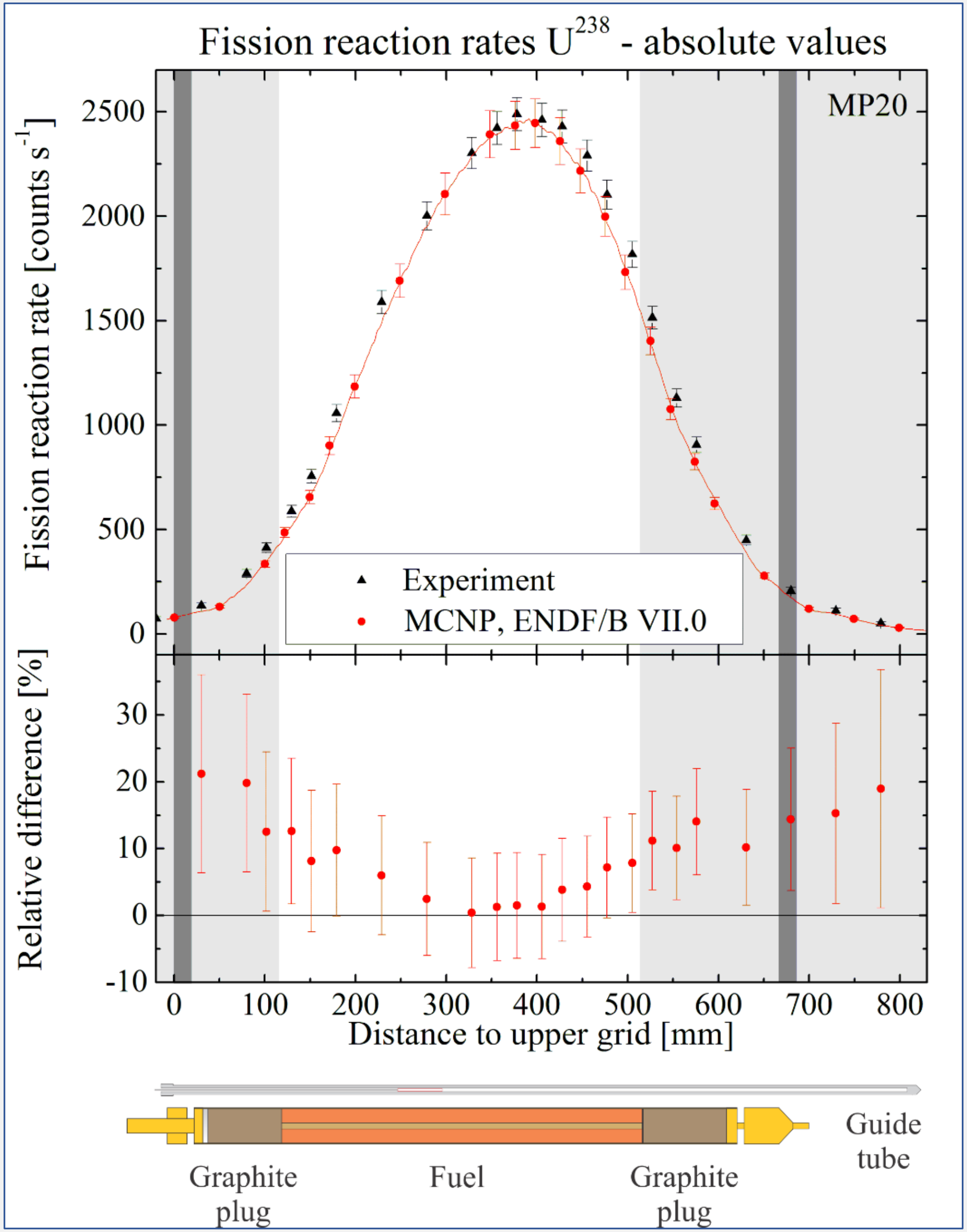
FISSION RATE AXIAL SCANS

Fission chamber

^{238}U (99.964 %)

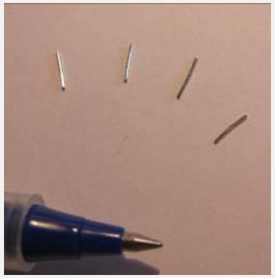
Reactor power:

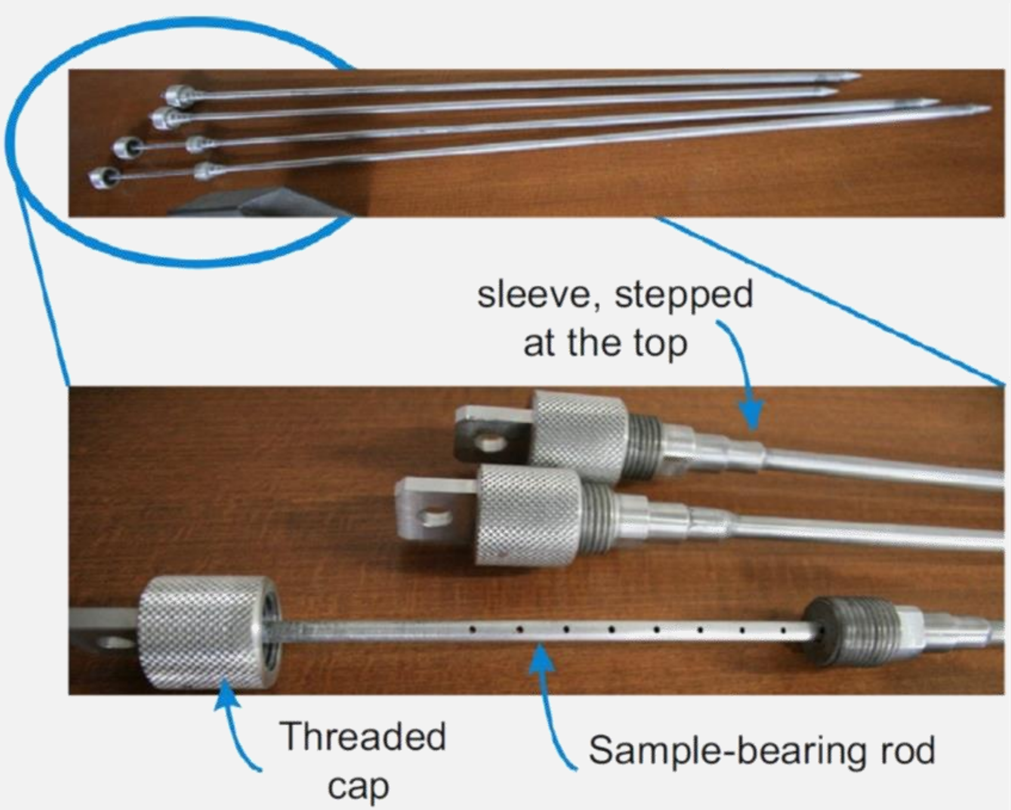
1000 W

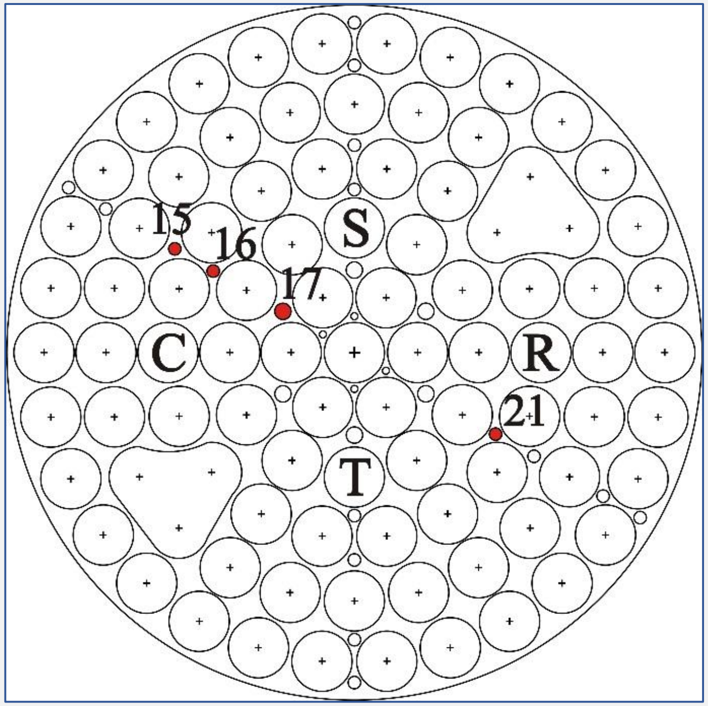


Au wires EXPERIMENT

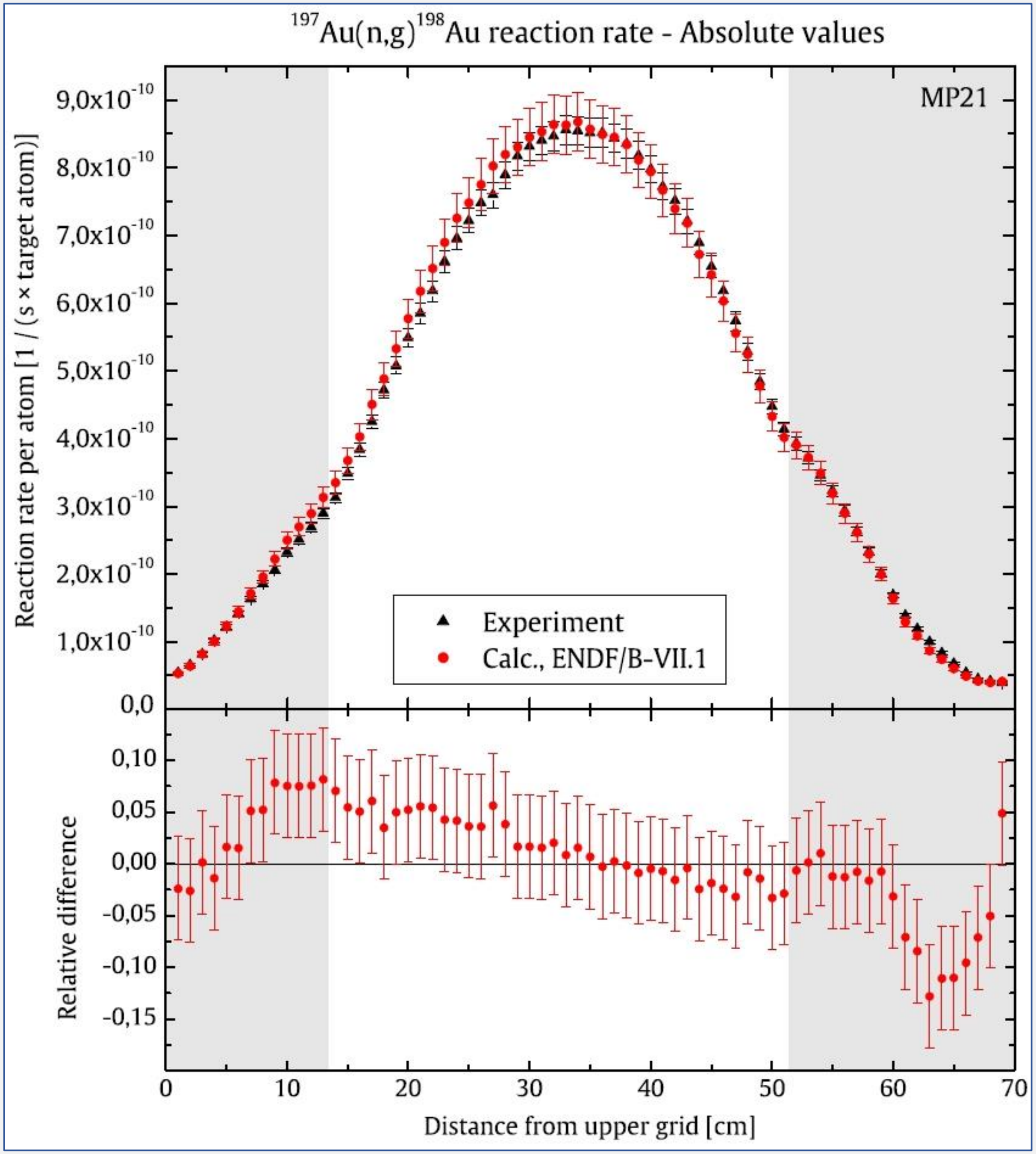
- Validational experiment using probes with Au wires
- Axial profiles of $^{197}Au\ (n,\gamma)\ ^{198}Au$ reaction rates







- Experimental and calculational Au reaction rates with relative discrepancies

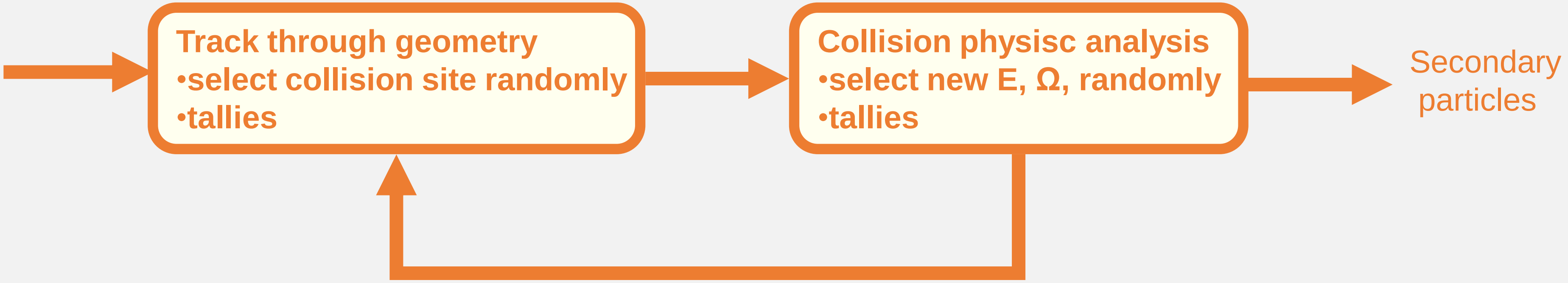


Monte Carlo neutron transport

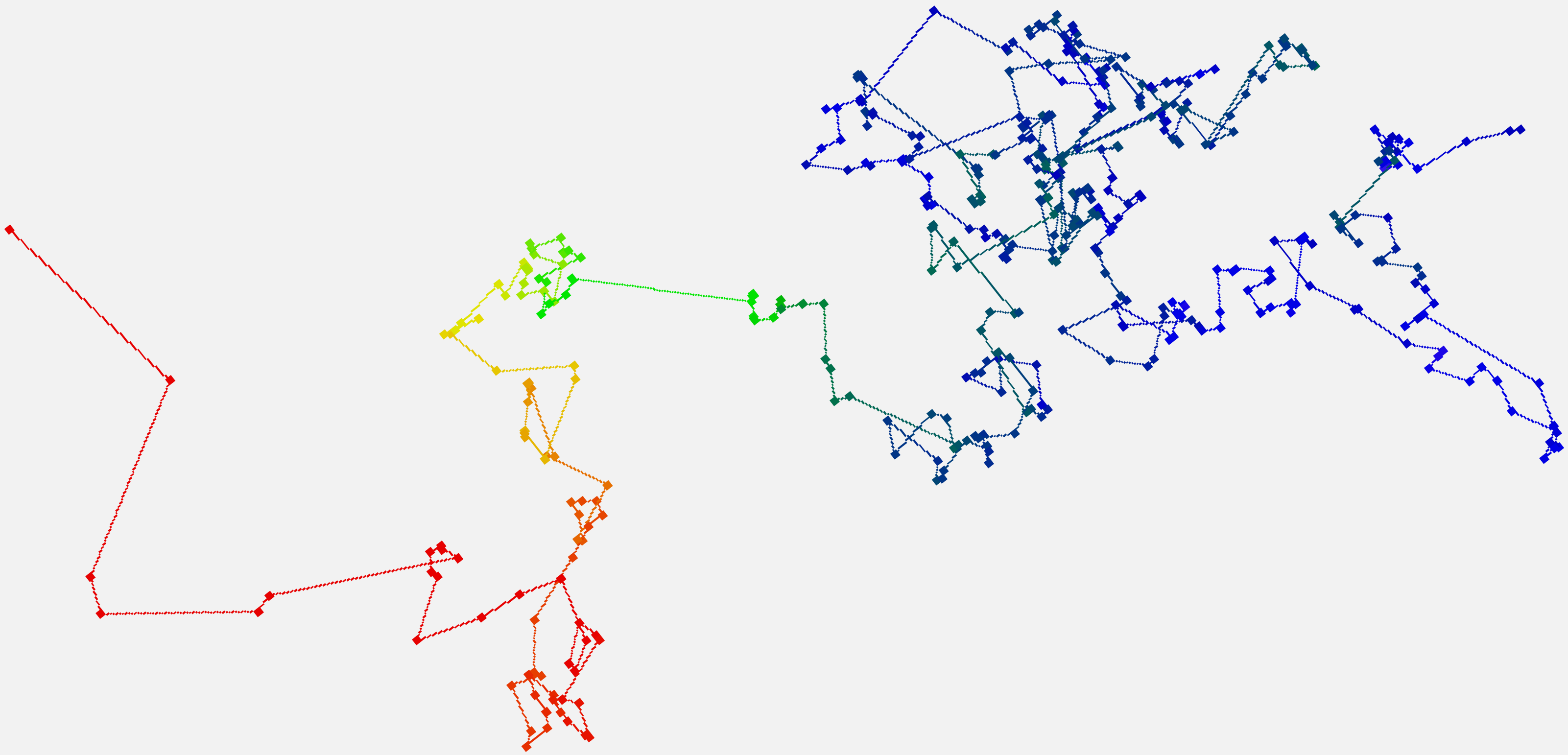
- Monte Carlo codes
  - **MCNP**, KENO, SERPENT, TRIPOLI, MCBEND, MONK, PHITS, OPENMC, SUPERMC, TART, COG, MCU,….
- Solving particle transport problems with the Monte Carlo method is simple – just simulate the particle behavior
- the problem lies in details: how to calculate reactor parameters, which are usually defined by deterministic (transport or difussion) methods

Monte Carlo simulation

- faithfully simulate the history of a single neutron from birth to death
- random walk for a single particle
  - model collisions using physics equation & cross section data
  - model free-flight between collisions using computational geometry
  - tally the occurrences of events (absorption, scattering, fission, track length,..) in each region
  - save any secondary particles, analyze them later

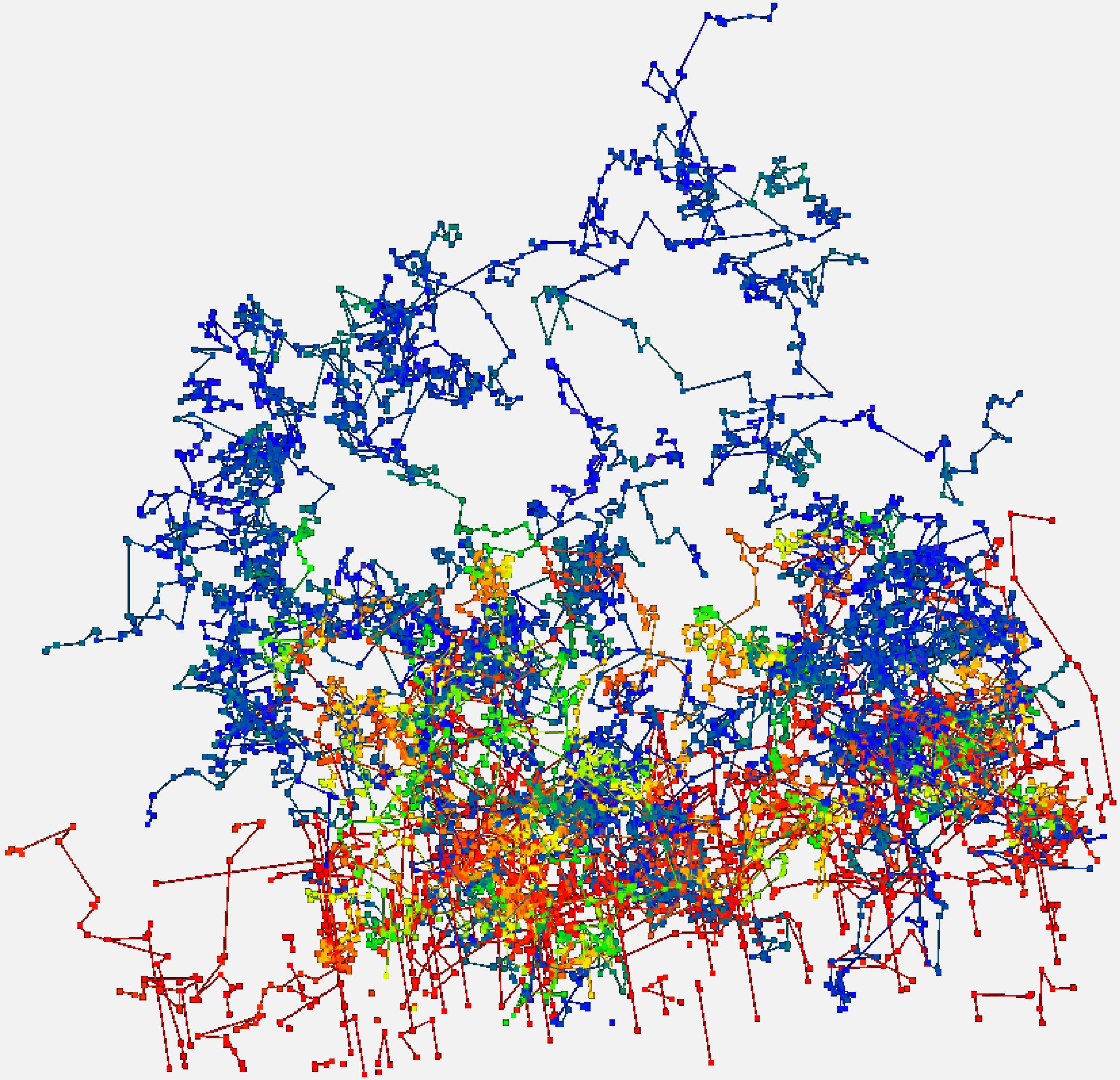


Neutron random walk



Monte Carlo histories

- Monte Carlo method for particle transport consists of simulating a finite number, say N, of particle histories through the use of a random number.
- In each particle history random numbers are generated and used to sample appropriate probability distributions for scattering angles, track length distances between collisions etc.
- $N \sim 10^6 - 10^{12}$



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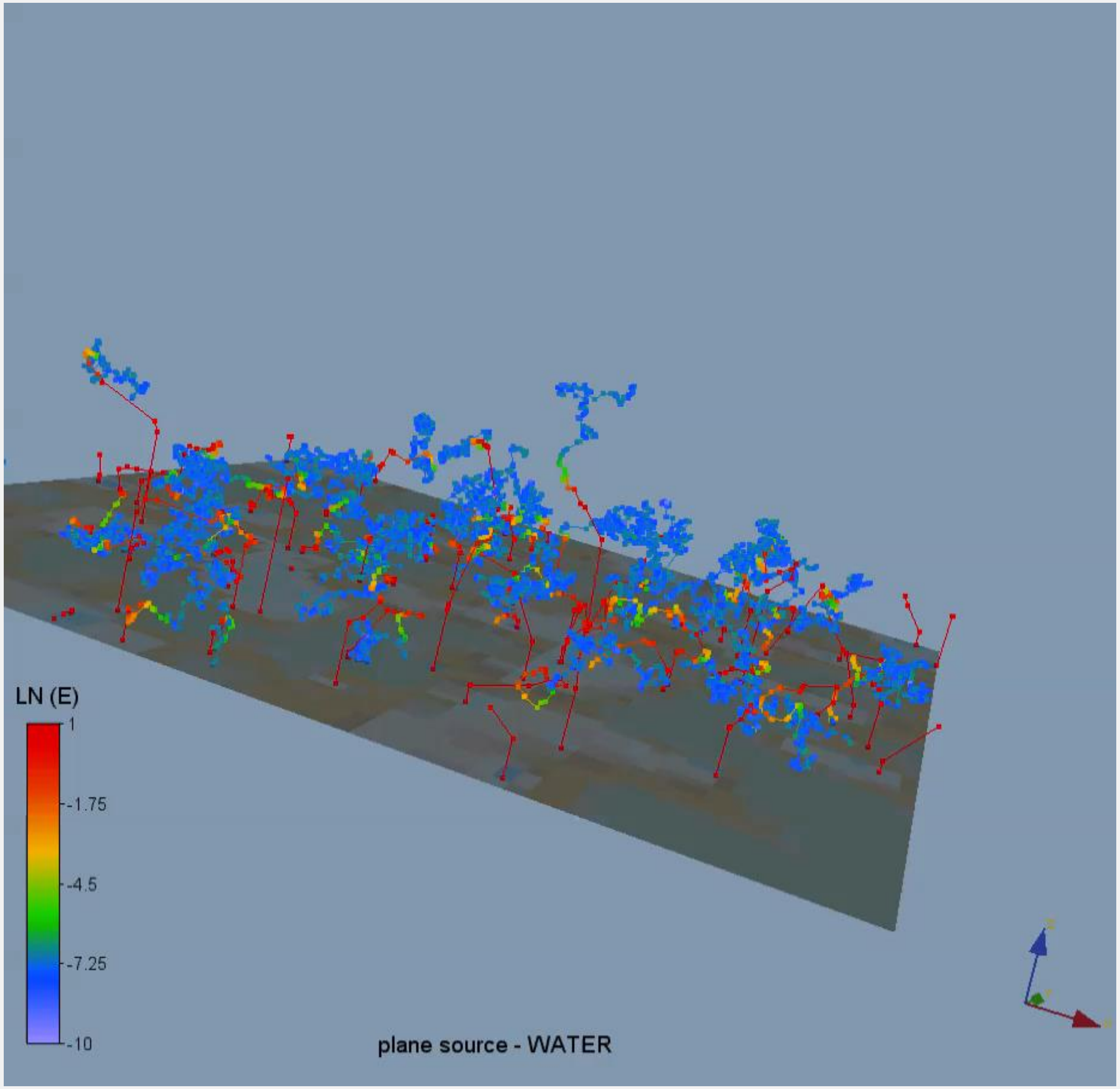
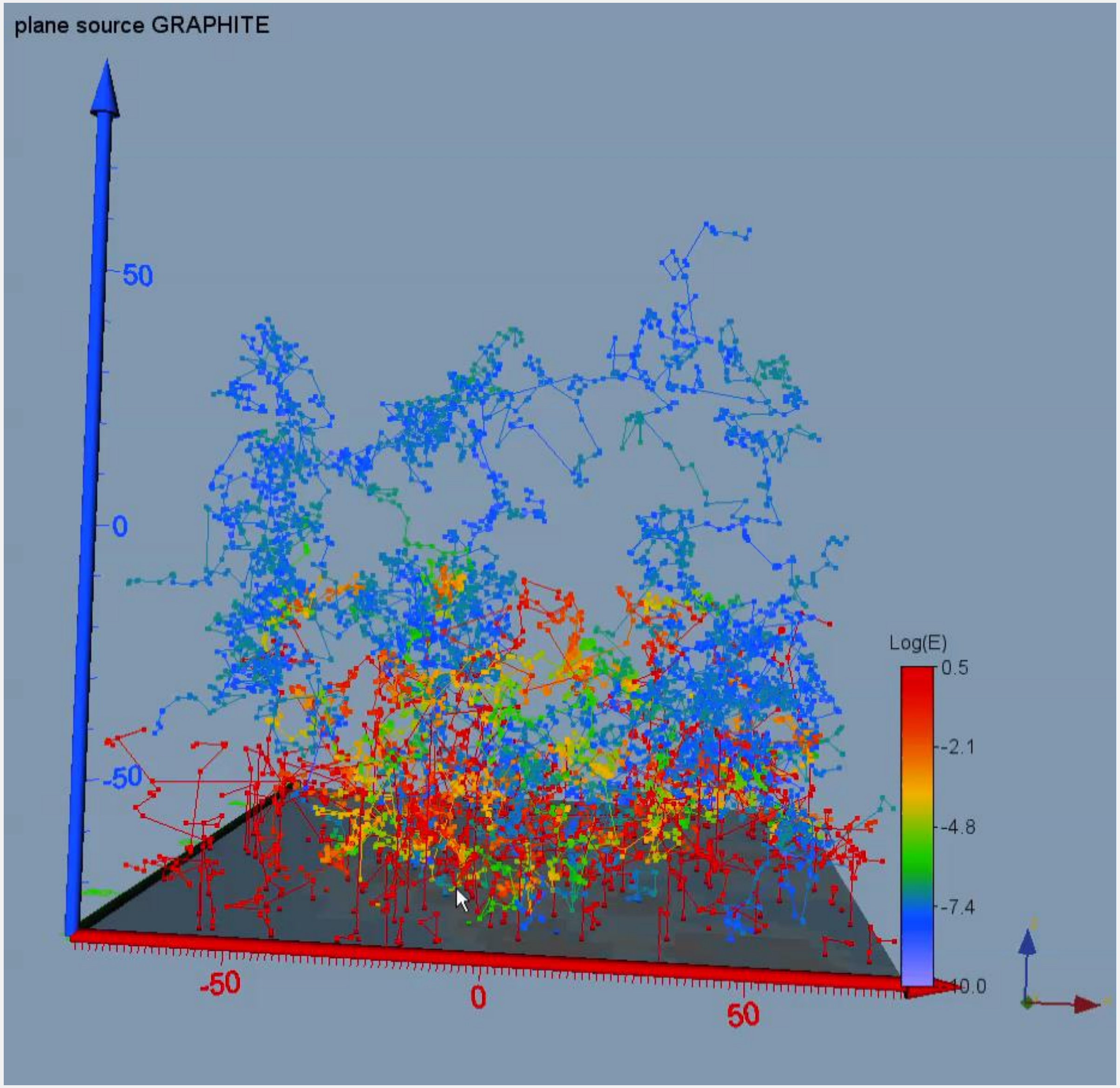
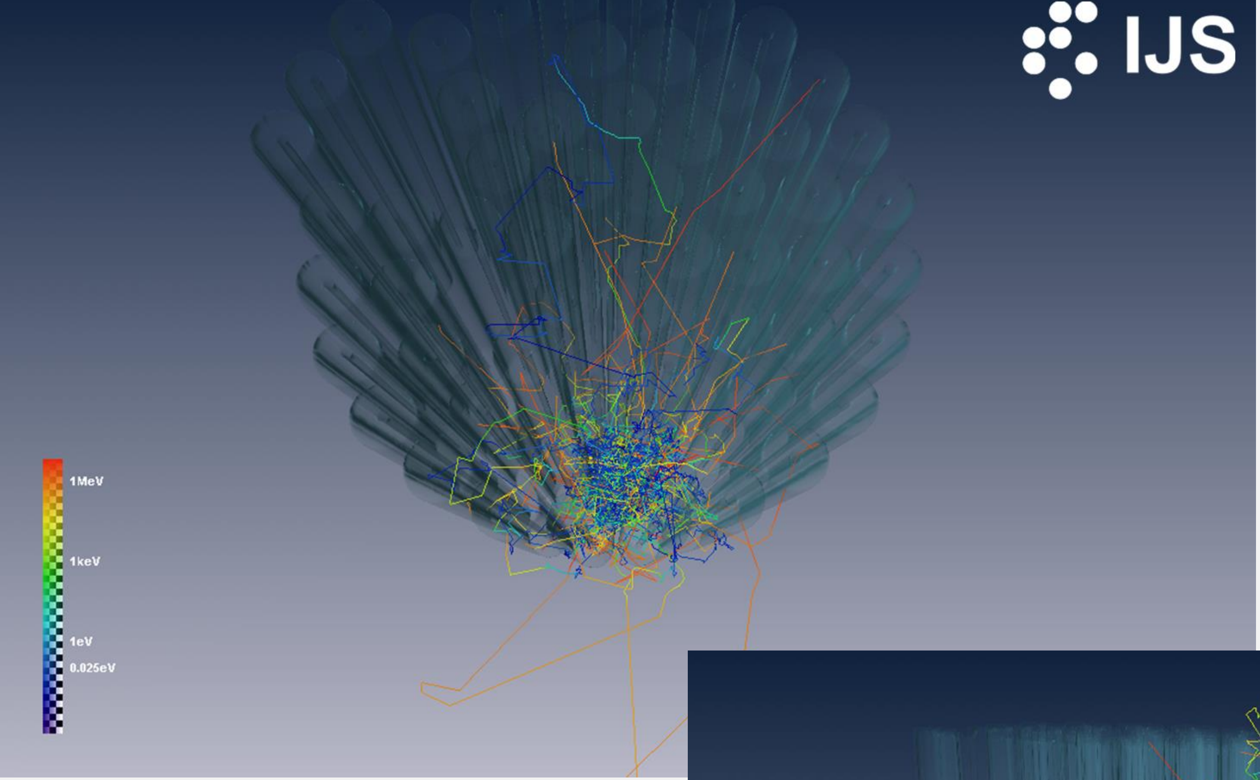
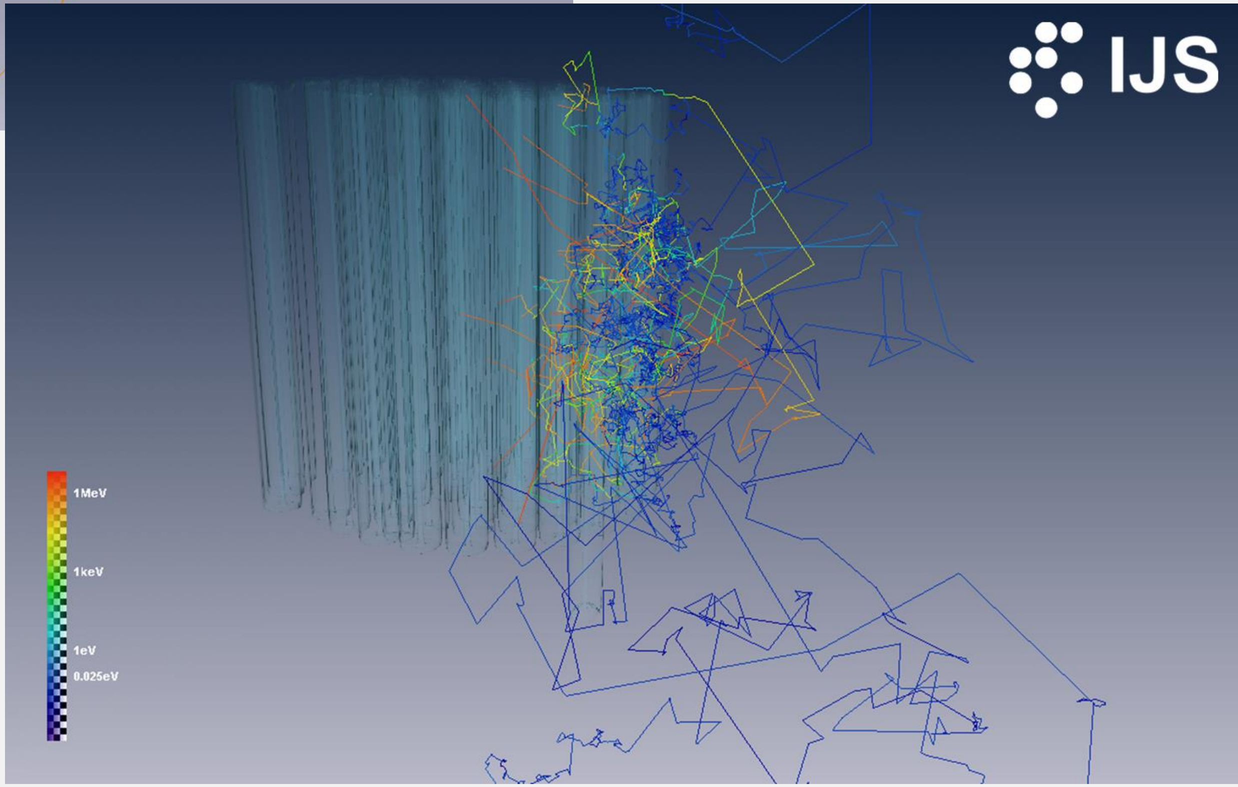
Particle tracks – water

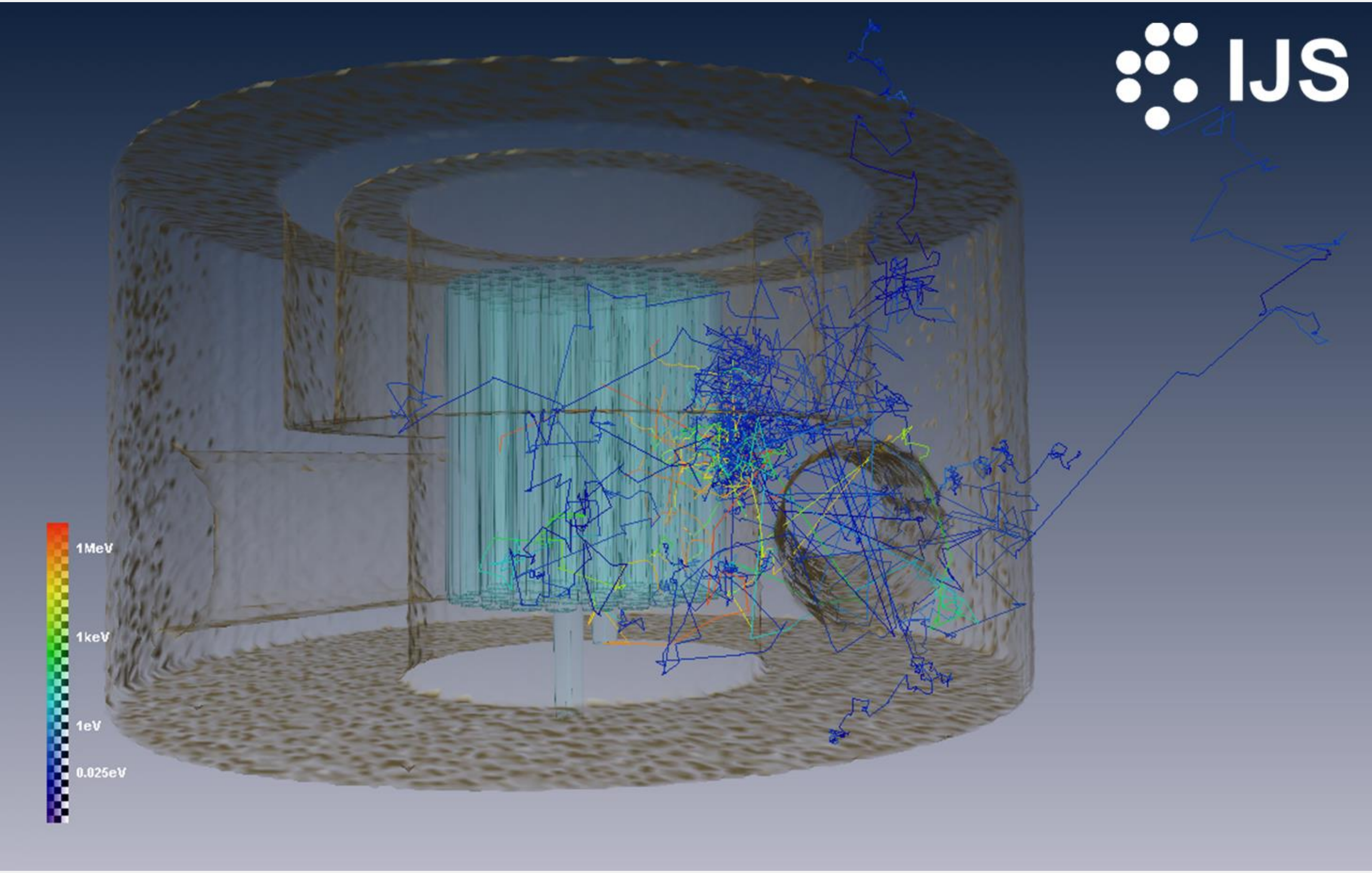


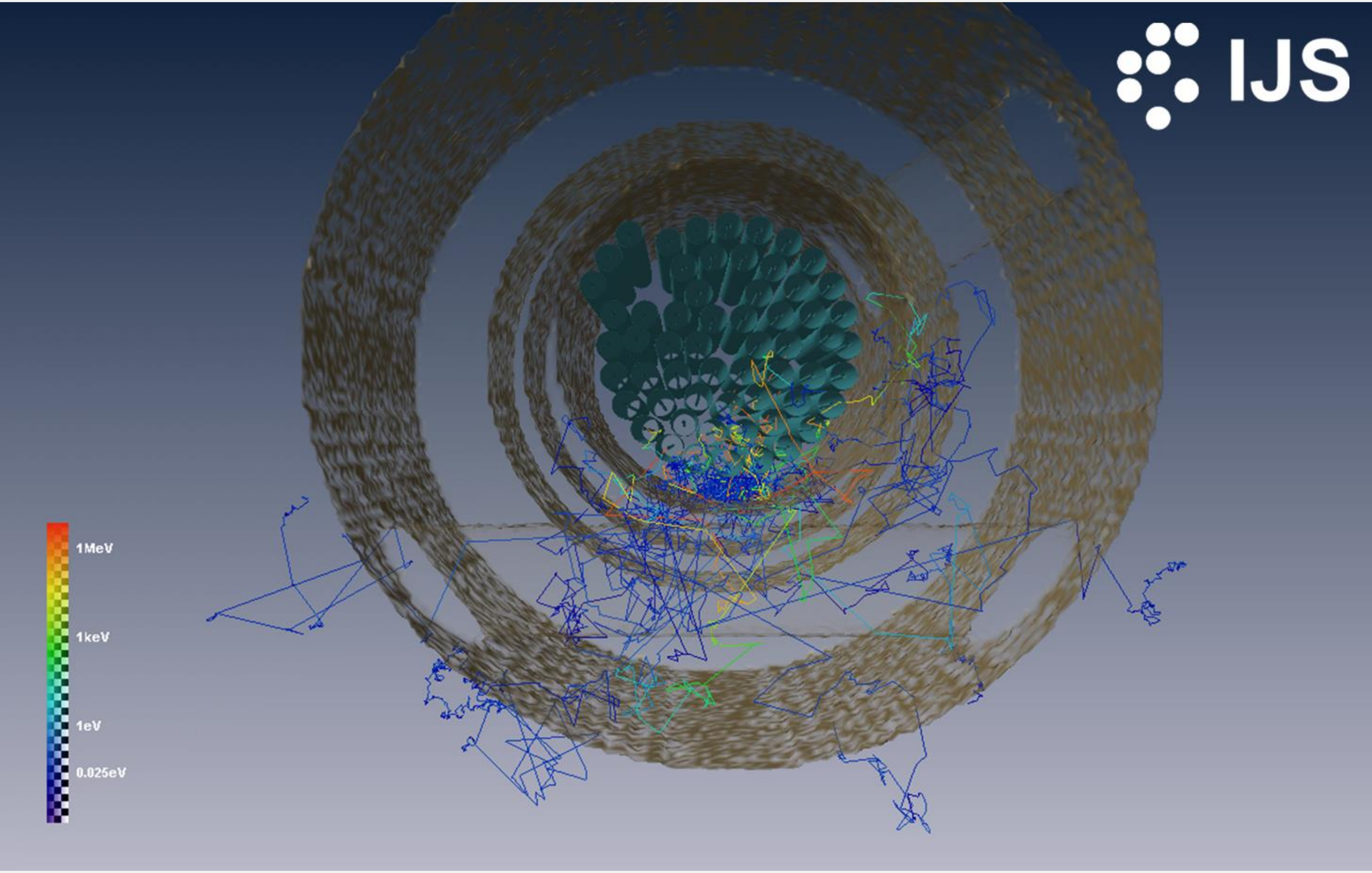
Particle tracks – graphite




IJS
1MeV
1keV
1eV
0.025eV

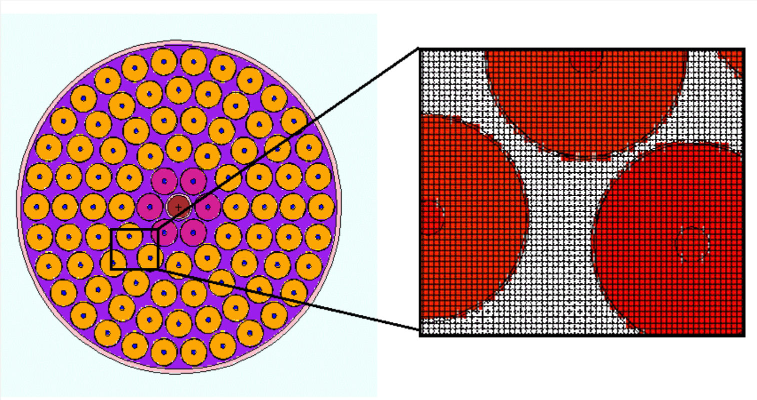

IJS
1MeV
1keV
1eV
0.025eV


1MeV
1keV
1eV
0.025eV

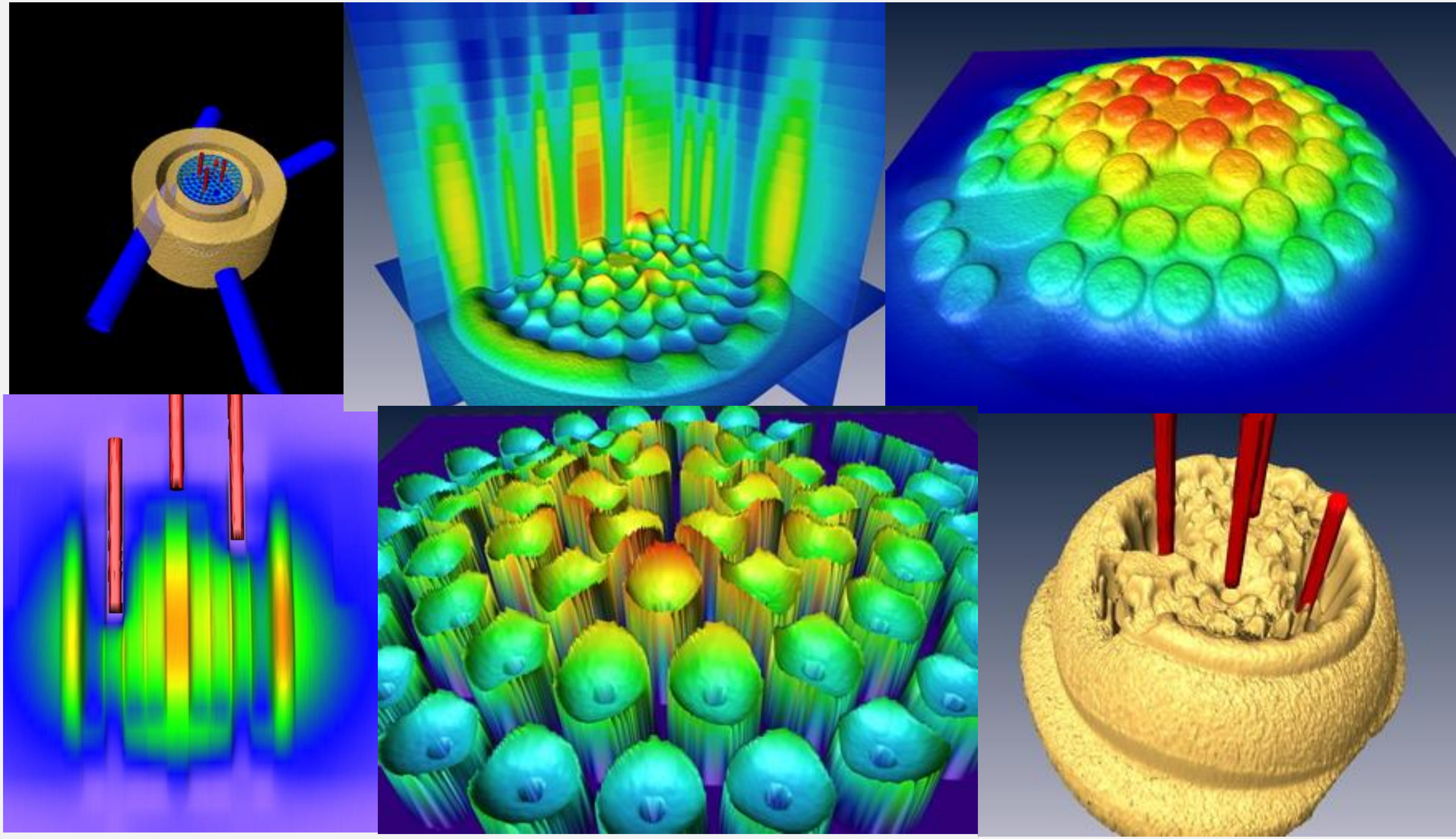

1MeV
1keV
1eV
0.025eV

Mesh tally

- very useful for calculation of
  - neutron flux distribution
  - power distribution
  - reaction rate distribution
- a mesh of cells is superimposed over the problem geometry
- useful also for
  - checking results
  - plotting problem geometry (advanced option)



Mesh tally – sample results



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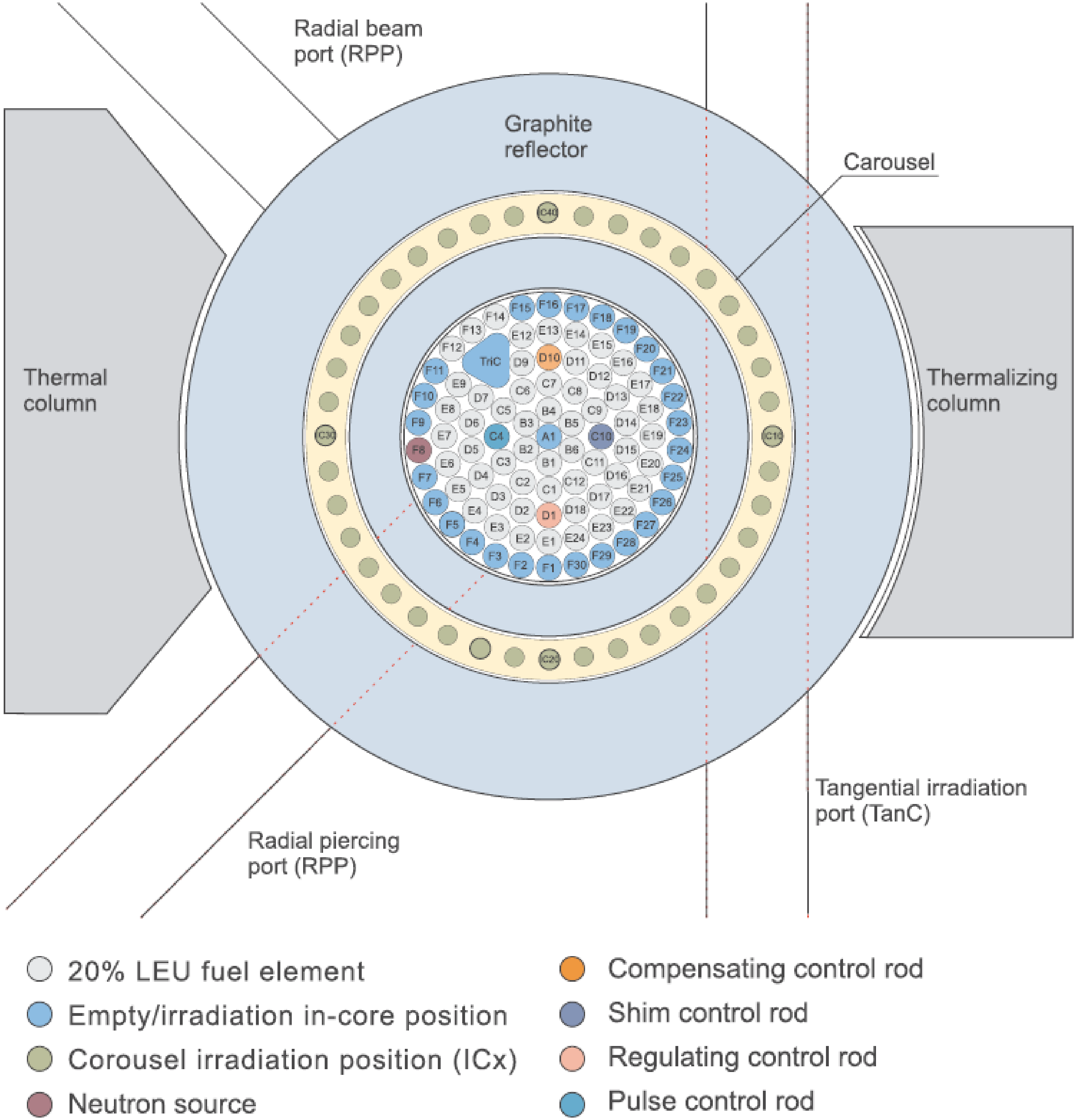
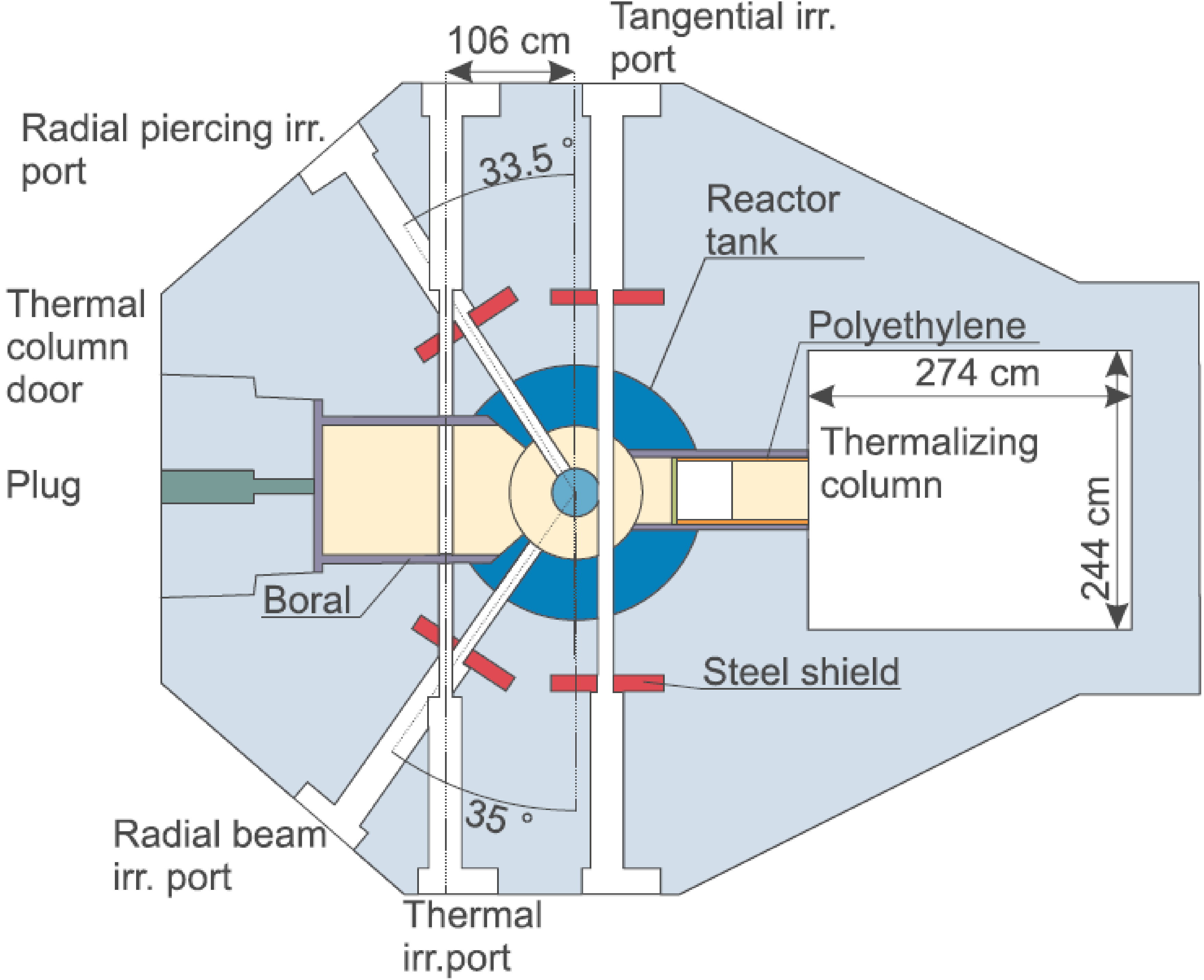
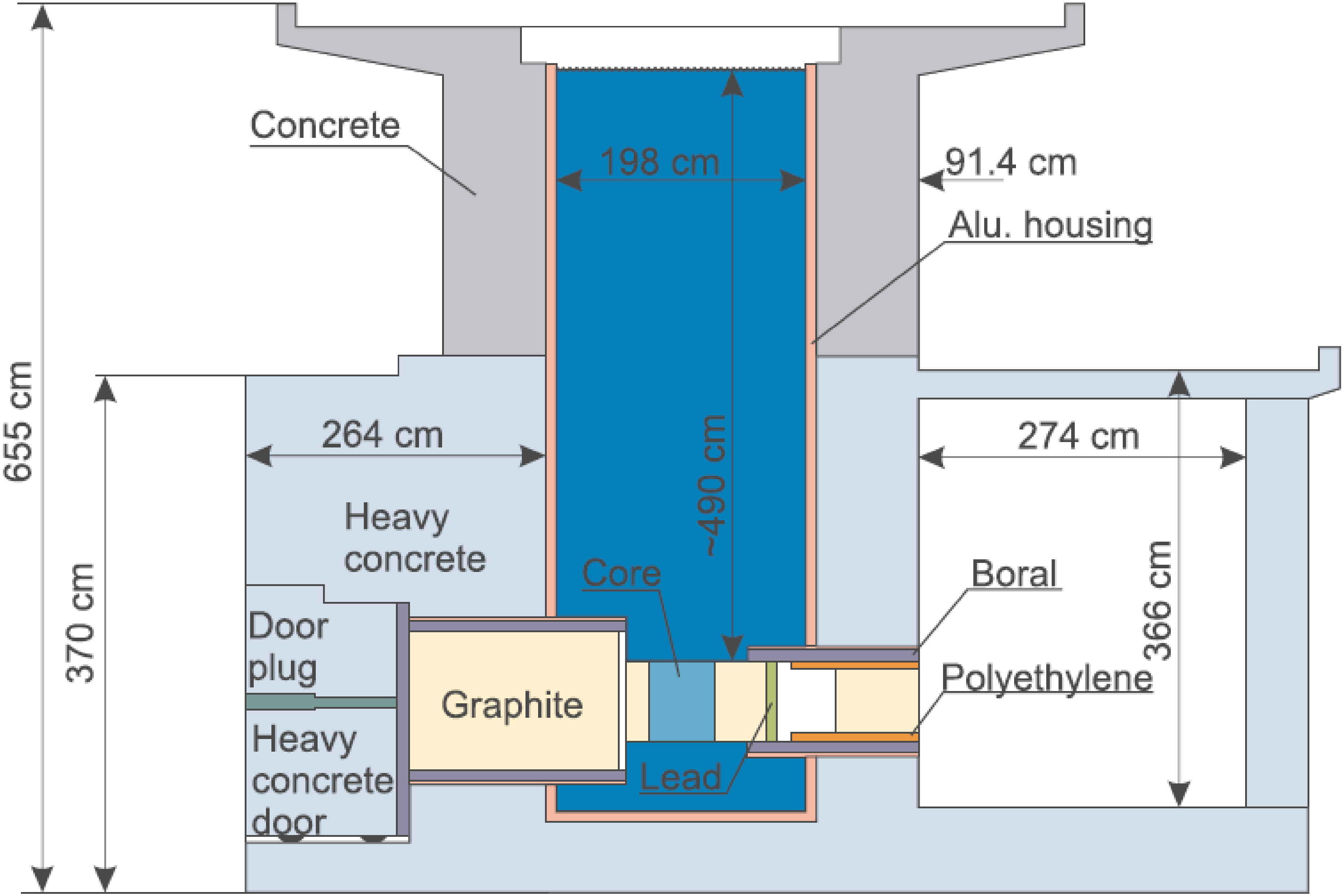
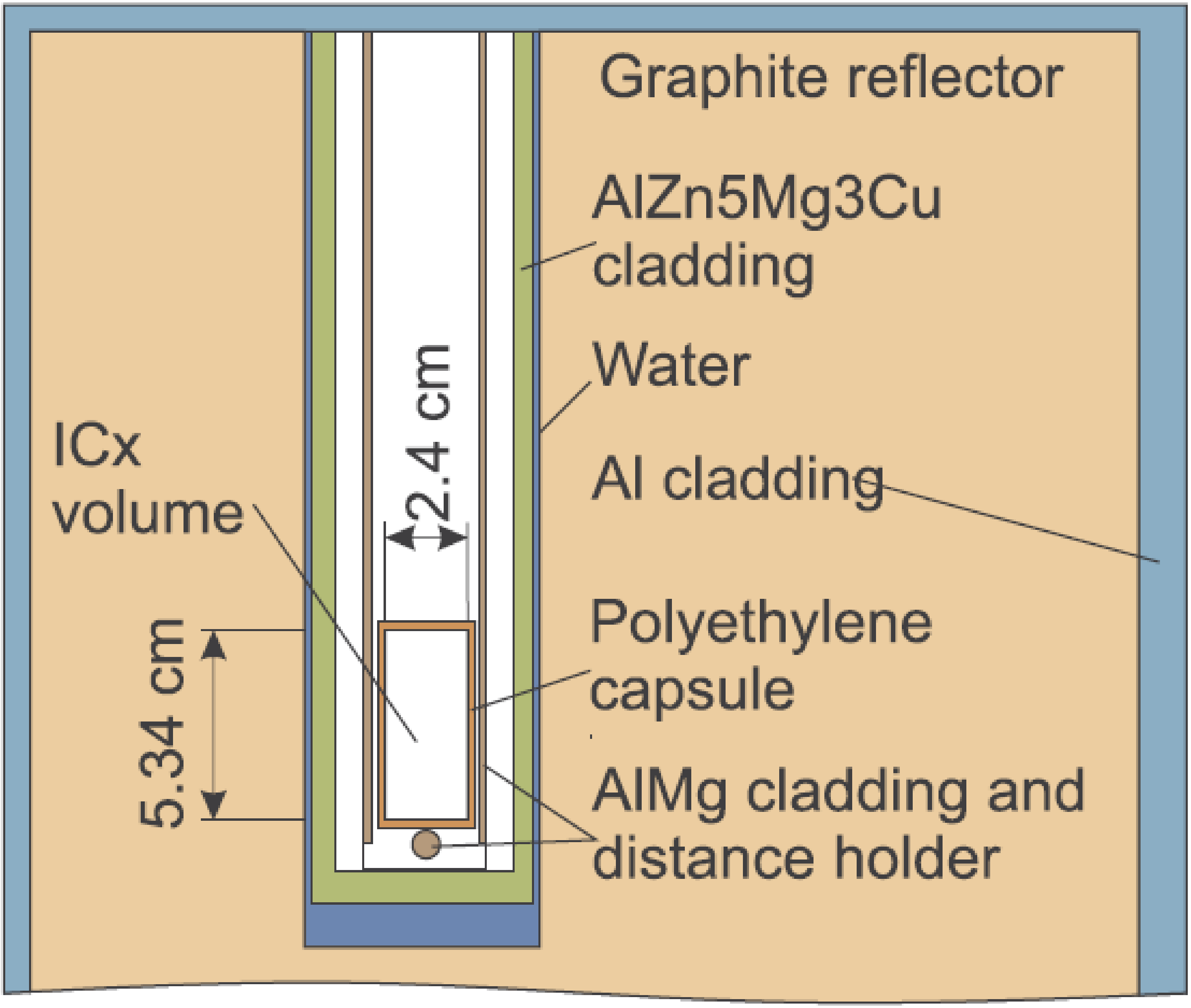

Radial beam port (RPP)
Graphite reflector
Carousel
Thermal column
Thermalizing column
Tangential irradiation port (TanC)
Radial piercing port (RPP)
20% LEU fuel element
Empty/irradiation in-core position
Corousel irradiation position (ICx)
Neutron source
Compensating control rod
Shim control rod
Regulating control rod
Pulse control rod

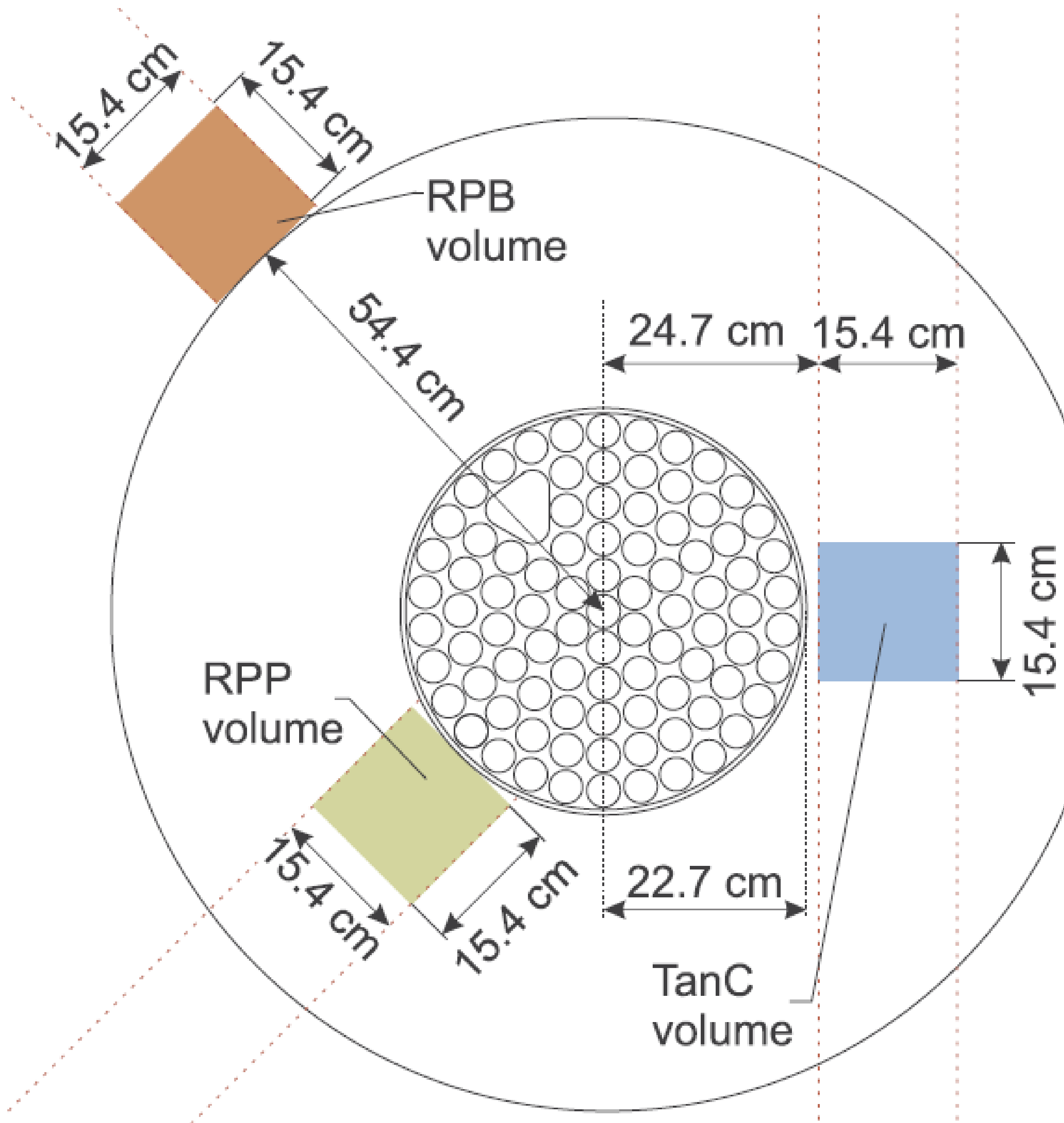


106 cm
Tangential irr. port
Radial piercing irr. port
33.5 °
Reactor tank
Thermal column door
Polyethylene
274 cm
Thermalizing column
Plug
244 cm
Boral
Steel shield
35 °
Radial beam irr. port
Thermal irr.port

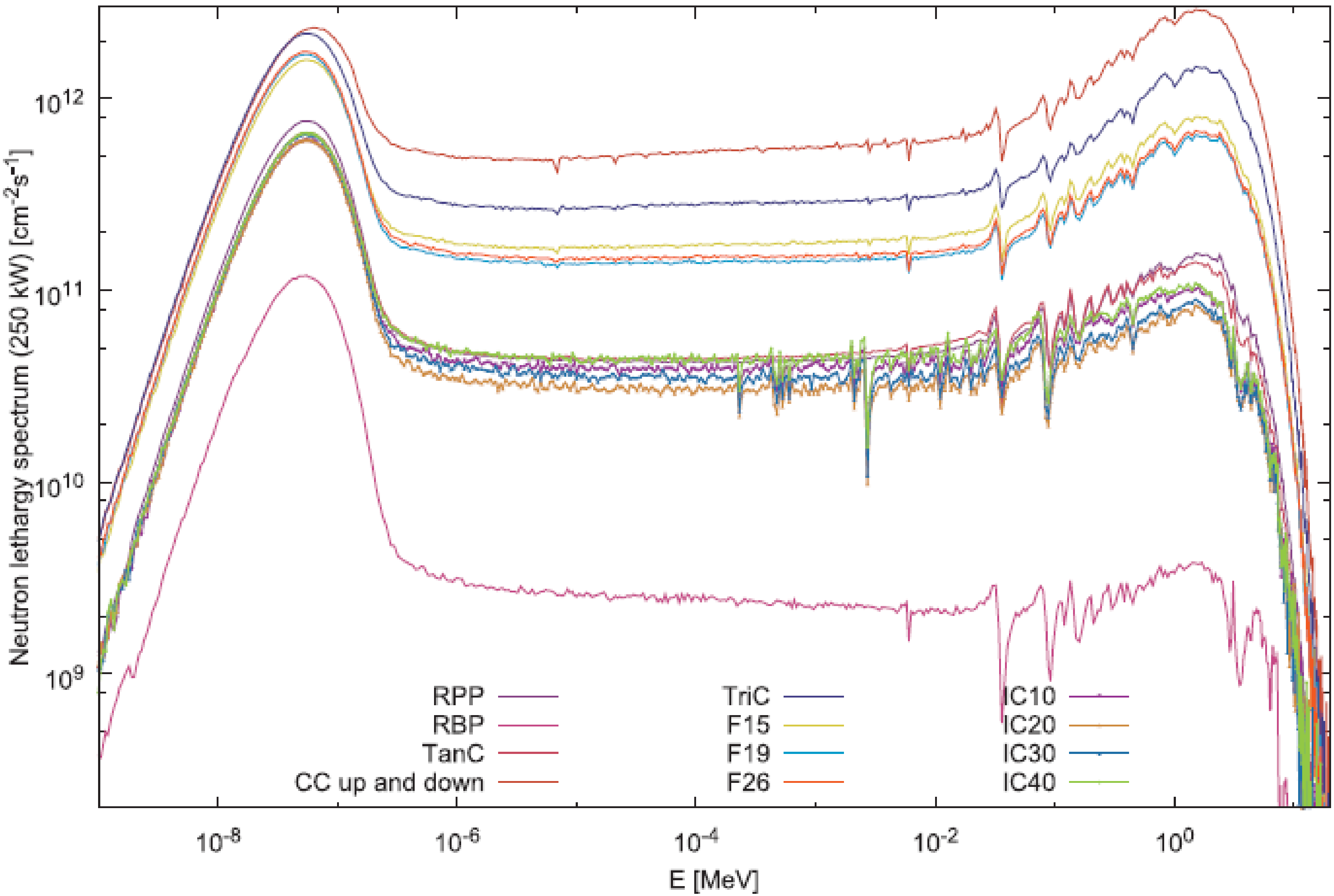


655 cm
370 cm
Concrete
198 cm
91.4 cm
Alu. housing
264 cm
~490 cm
274 cm
Heavy concrete
Core
Boral
366 cm
Door plug
Graphite
Polyethylene
Heavy concrete door
Lead

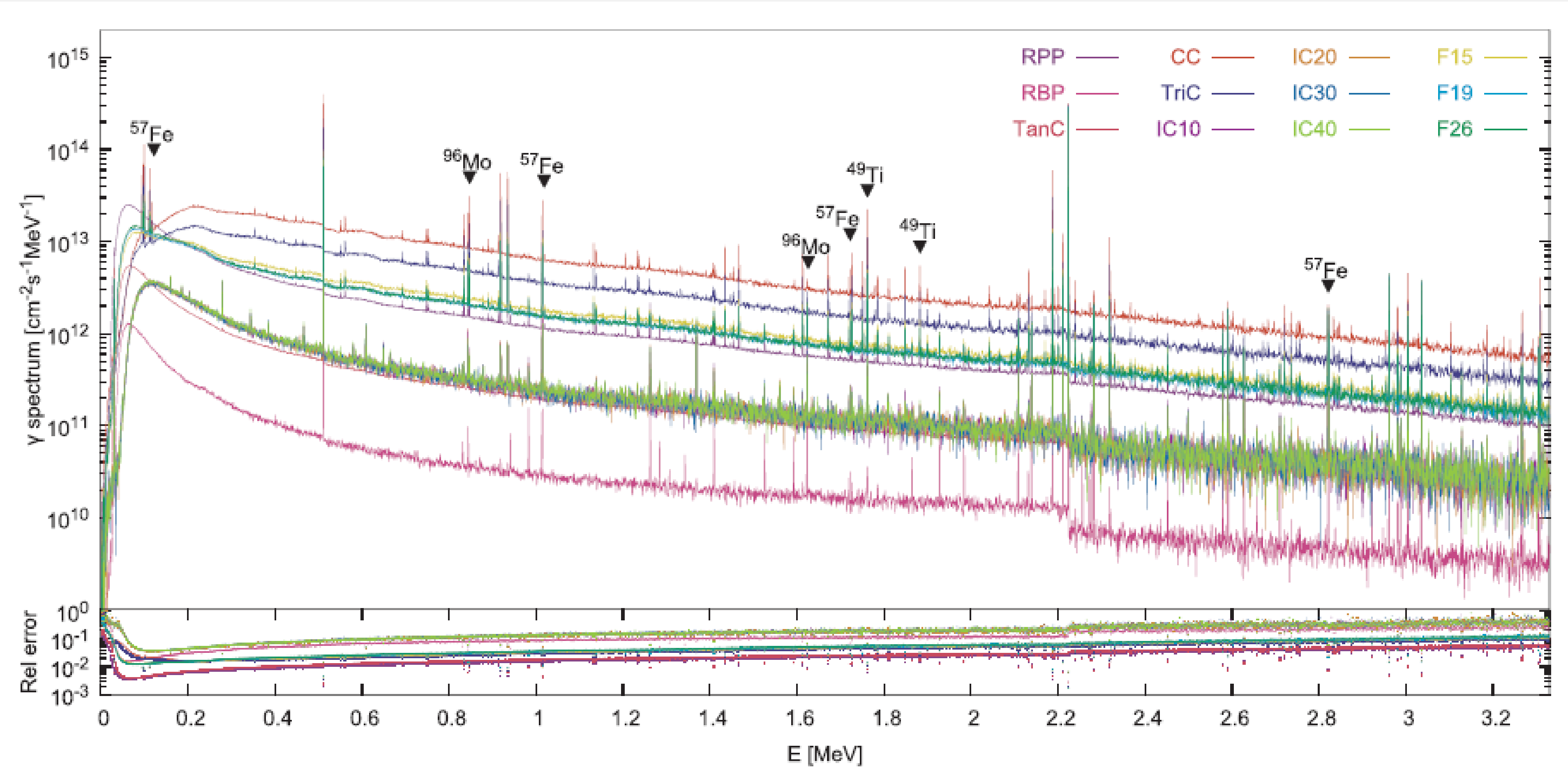

Graphite reflector
AlZn5Mg3Cu cladding
Water
Al cladding
ICx volume
2.4 cm
5.34 cm
Polyethylene capsule
AlMg cladding and distance holder


15.4 cm
15.4 cm
RPB
volume
54.4 cm
24.7 cm
15.4 cm
15.4 cm
RPP
volume
15.4 cm
15.4 cm
22.7 cm
TanC
volume

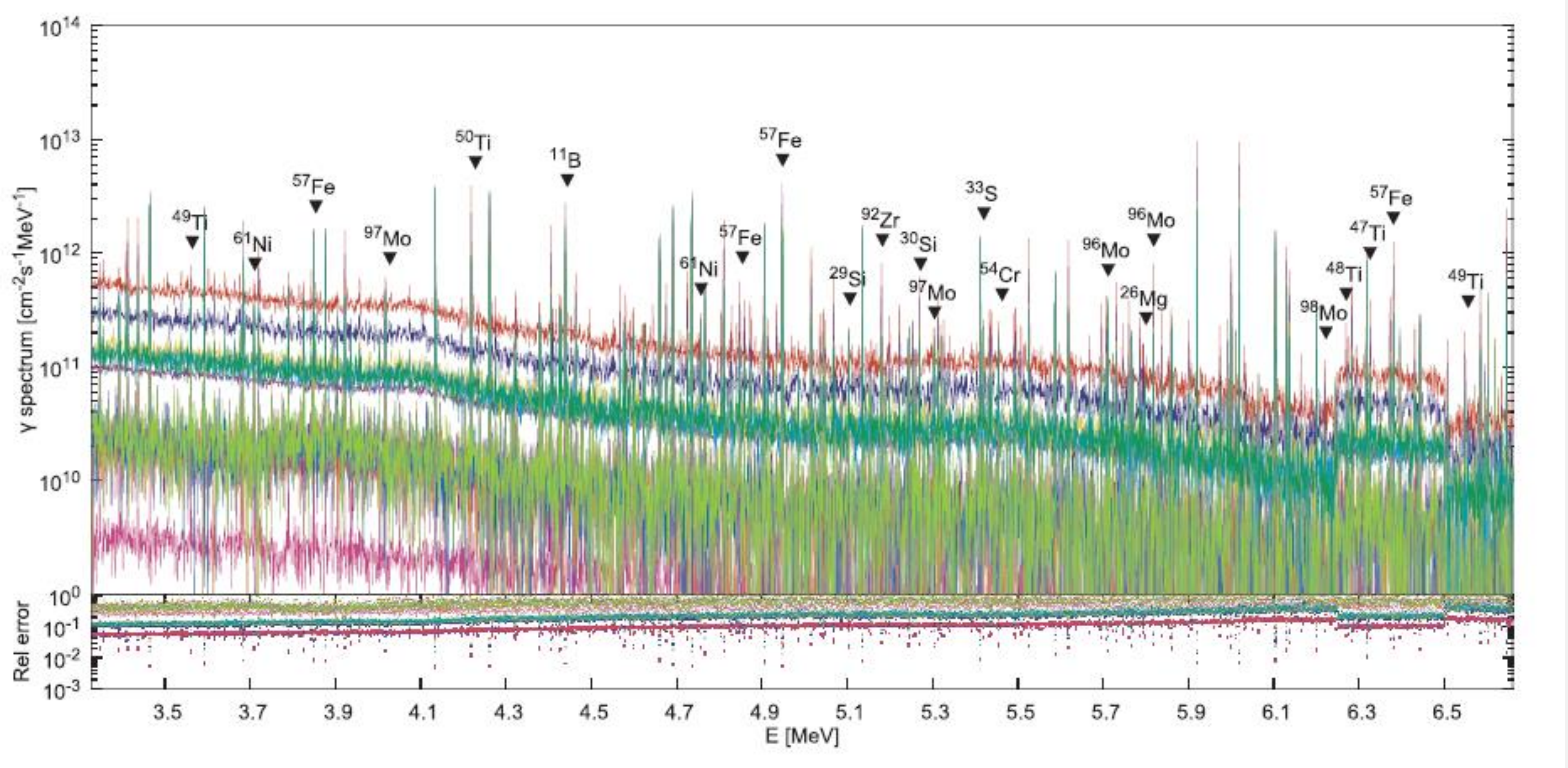
Neutron flux spectrum



Gamma spectrum (0 – 3.3) MeV



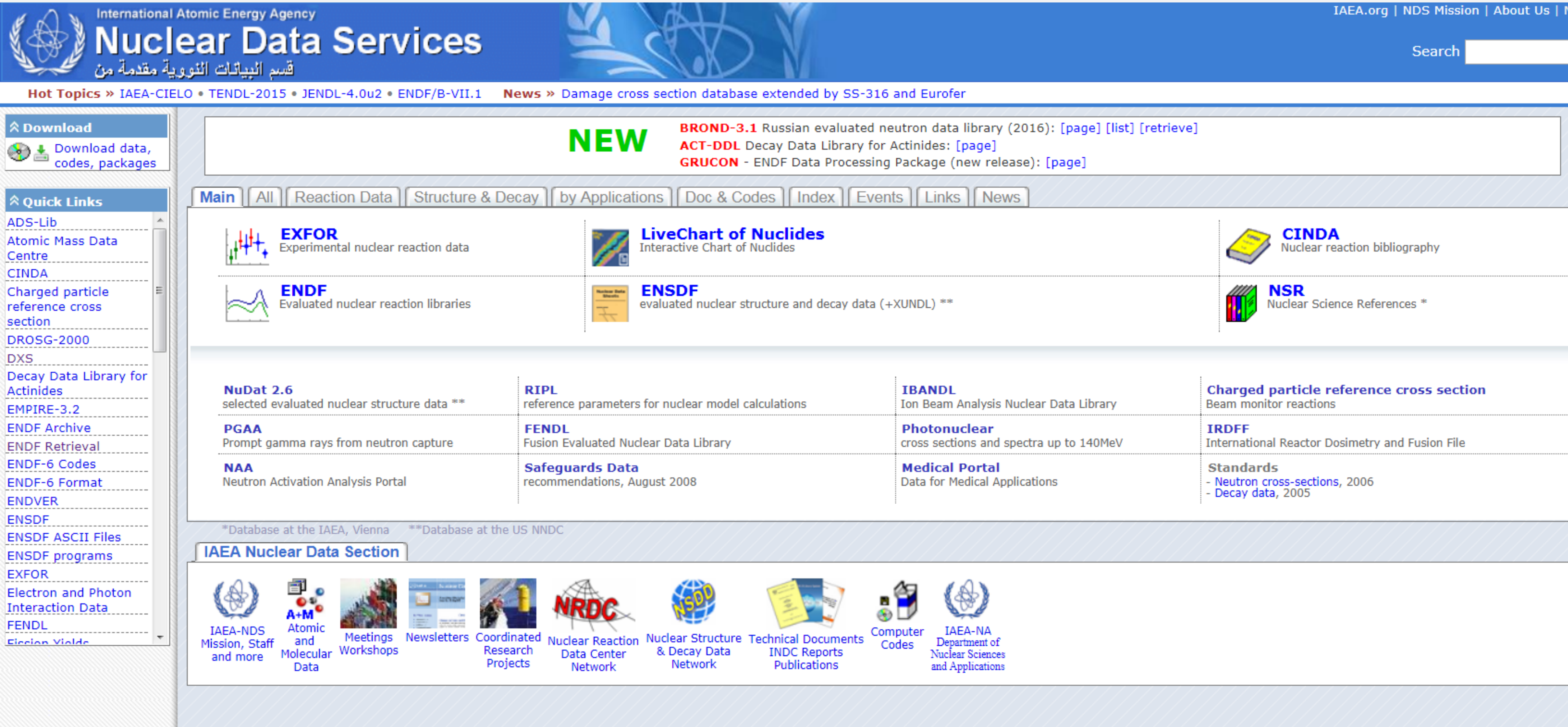
Gamma spectrum (3.3-6.6) MeV



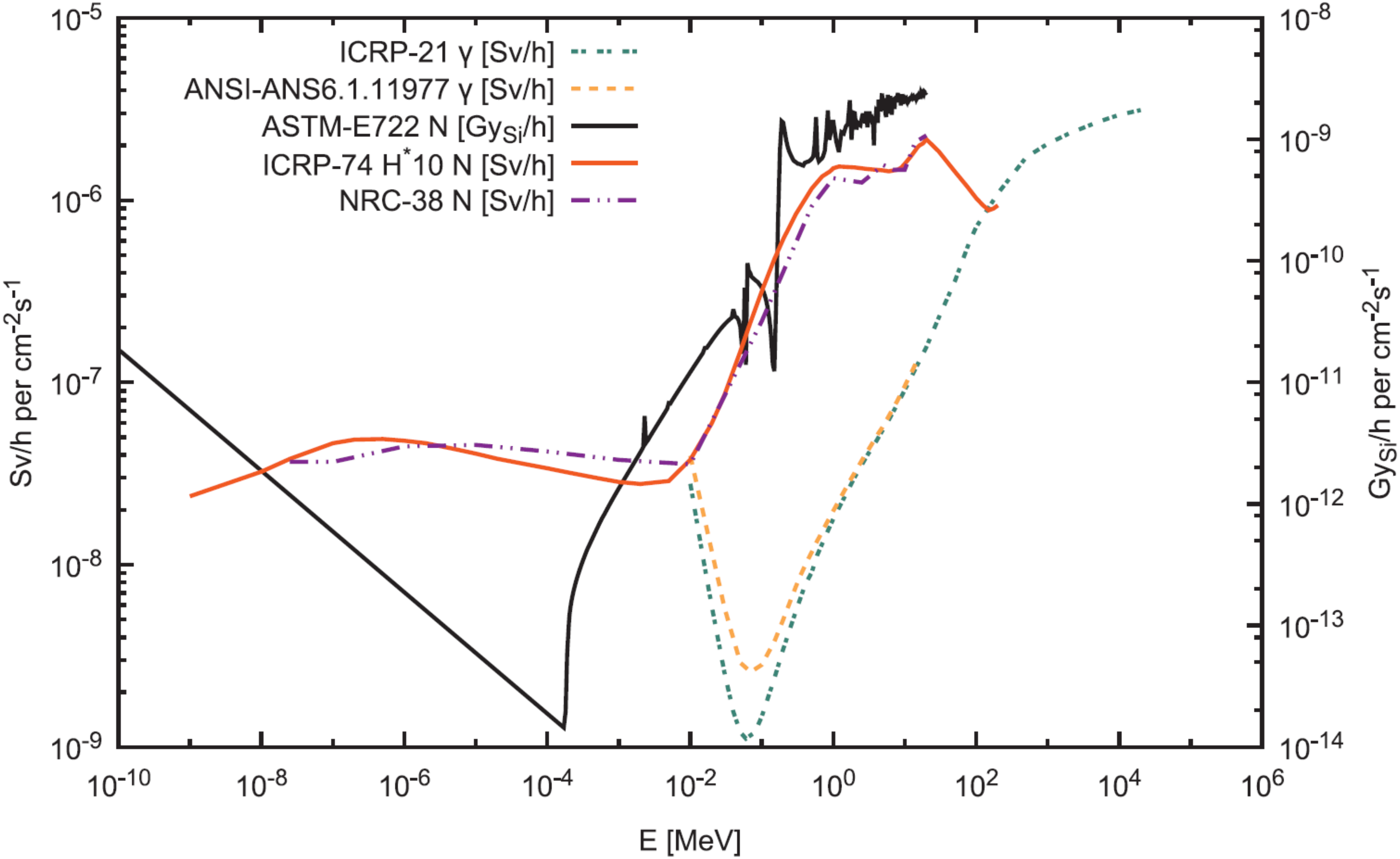
Nuclear data

$$\text{reaction rate} = \sigma\,\varphi = \int \sigma(E)\varphi(E)\,dE$$

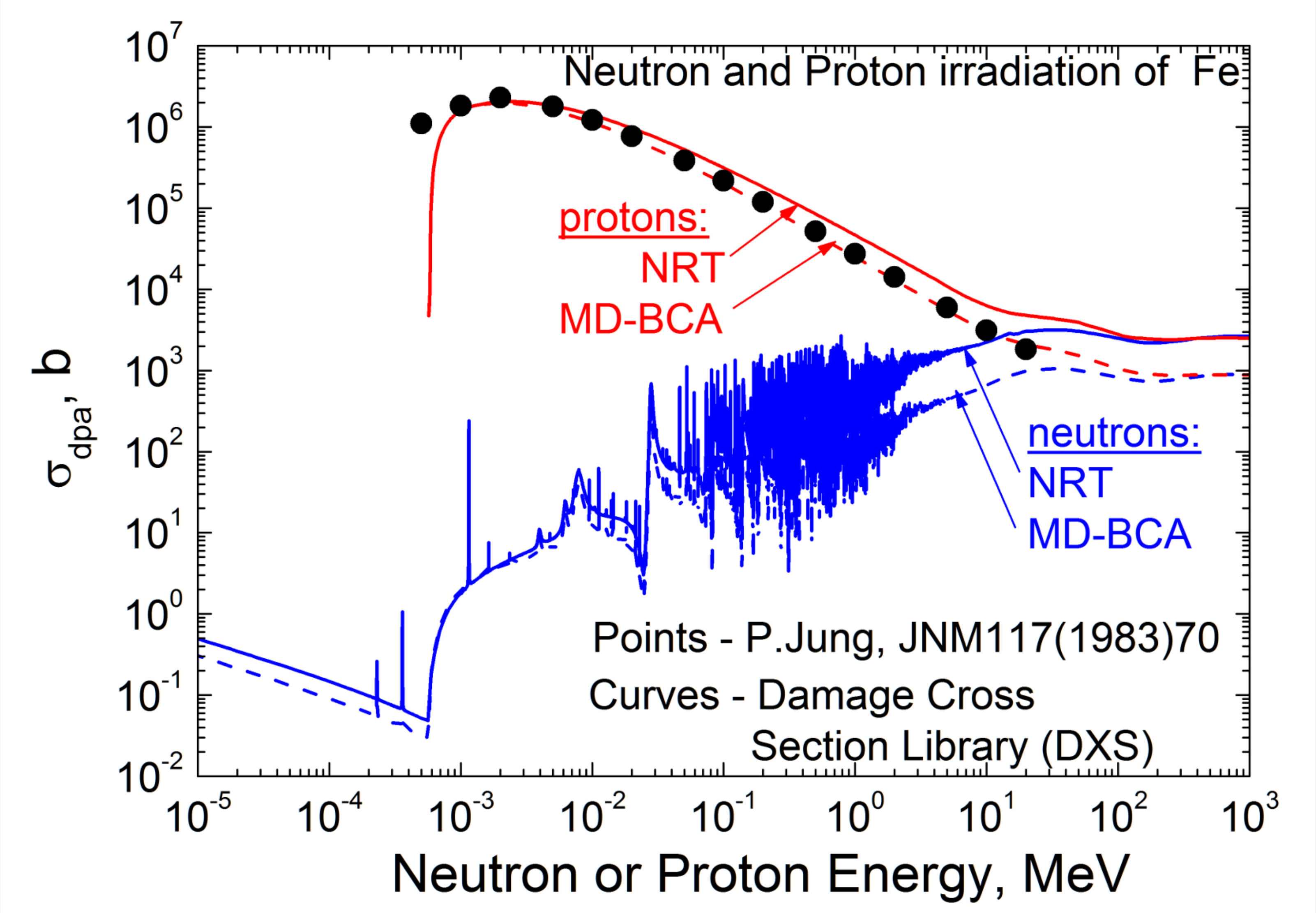
- Source: https://www-nds.iaea.org



Flux to dose conversion factors



DPA –displacement per atom



https://www-nds.iaea.org/dpa/

Conclusion

- RR calculations
  - Reduce time required to optimise experiments
  - Provide insight into reactor physical parameter not possible by experiments
  - Provide large amounts of data in relatively short time
- RR codes and models should be verified and validated by experiments

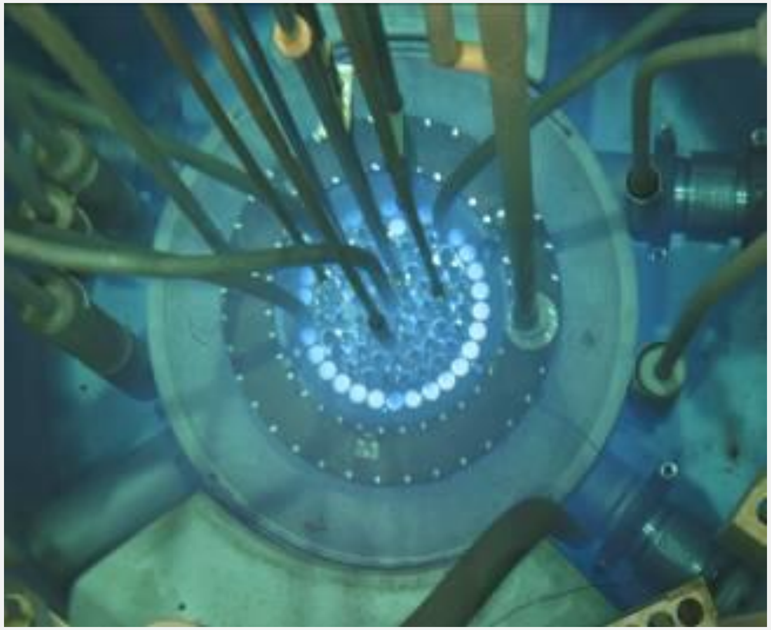
RR simulator

- WWW: http://reactorsimulator.ijs.si
- @: reactor-simulator@ijs.si

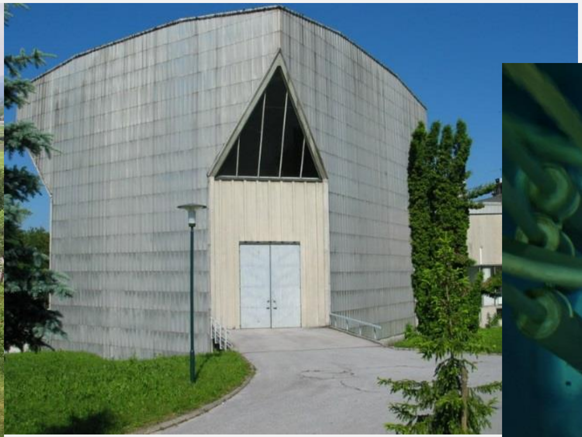
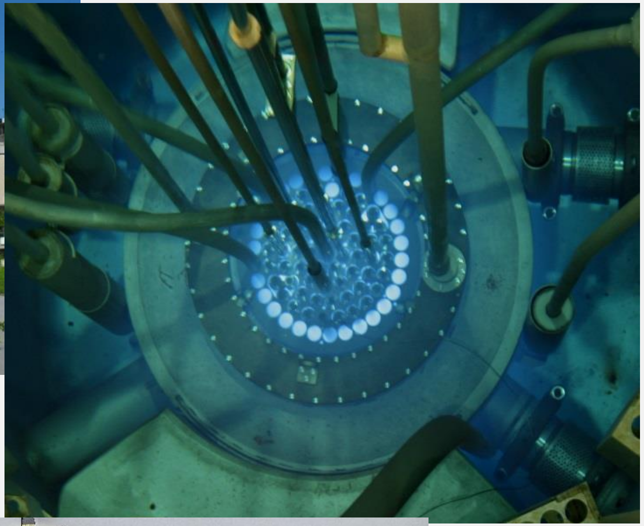
Additional slides

Jožef Stefan Institute TRIGA reactor

- 1st criticality: 31st May, 1966
- P_{max}
  - 250 kW (steady state)
  - 1 GW (pulse)
- Fuel rod
  - UZrH (m~2300 g)
  - 12 wt. % U
  - 20 % enriched U
  - (m (^{235}U) ~ 56 g)
  - SS cladding (h = 55cm, r = 1.8 cm)



TRIGA Mark II Reactor Ljubljana

- 1st criticality: 31st May, 1966
- P_{max}
  - 250 kW (steady state)
  - 1 GW (pulse)
- Fuel
  - UZrH (12 wt. % U)
  - E= 20 %

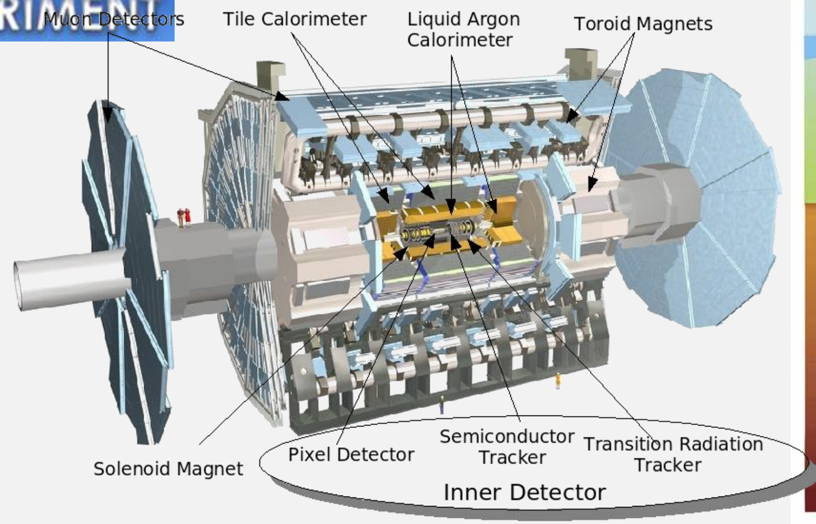
Present utilisation

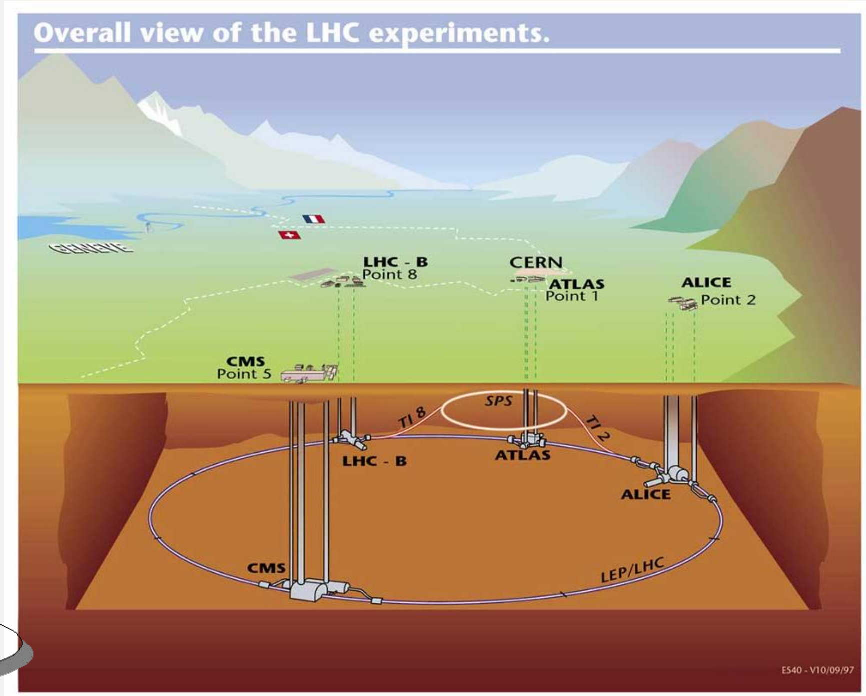
- research
  - verification and validation of computer codes and nuclear data – experimental benchmarks
  - testing and development of experimental equipment used for core physics tests at the Krško Nuclear Power Plant
  - testing of nuclear instrumentation (SPND, SPGD, miniature FC)
  - radiation hardness studies
- neutron activation analysis
- training (domestic + international courses)

Radiation hardness studies

- since 2001
- ~2000 samples/y, CERN, DESY, KEK and various universities and institutes.
- Neutron and gamma testing

ATLAS EXPERIMENT





AIDA 2020 Advanced European Infrastructures for Detectors at Accelerators

Benchmark

noun

a standard or point of reference against which things may be compared

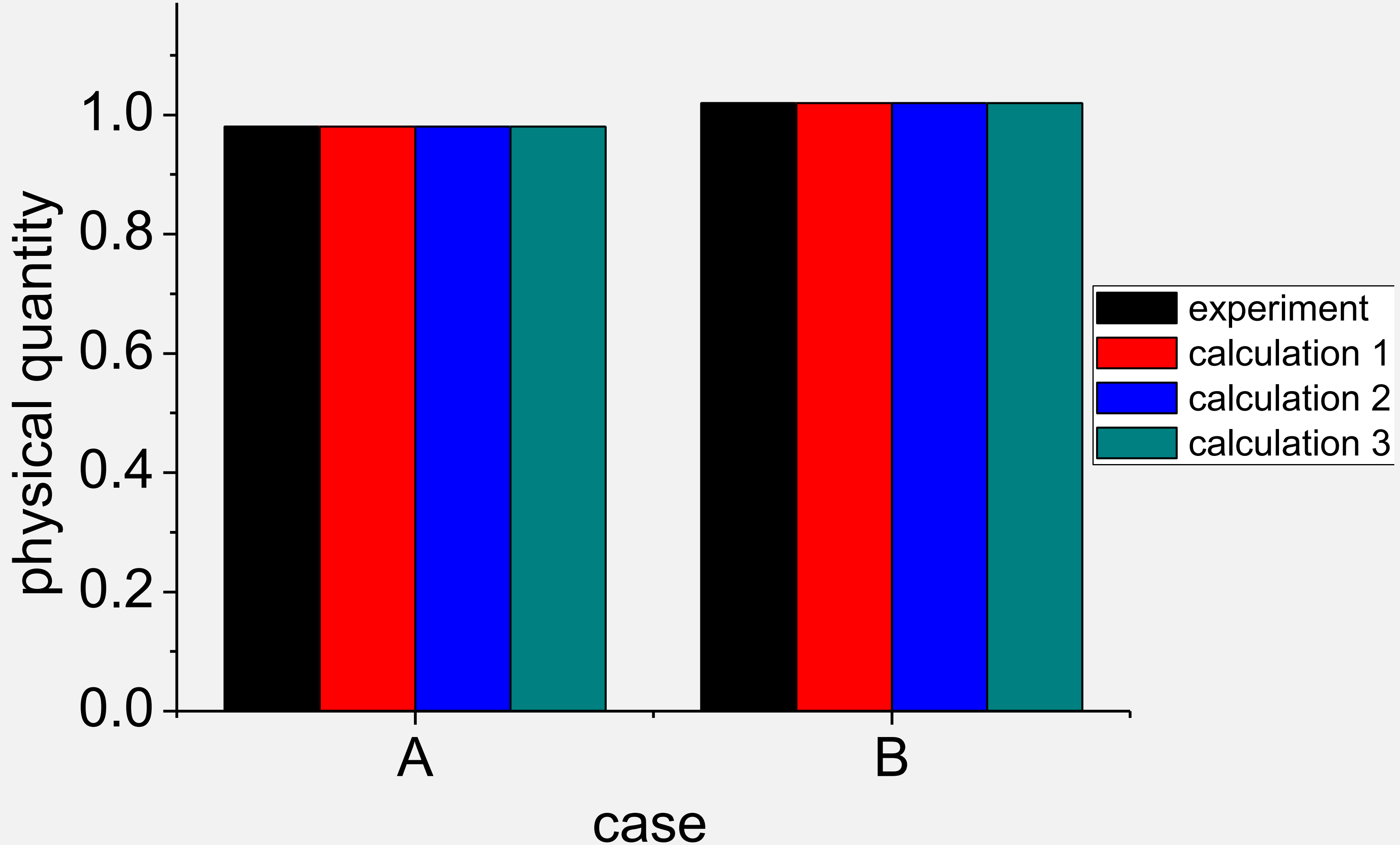
verb

evaluate (something) by comparison with a standard.

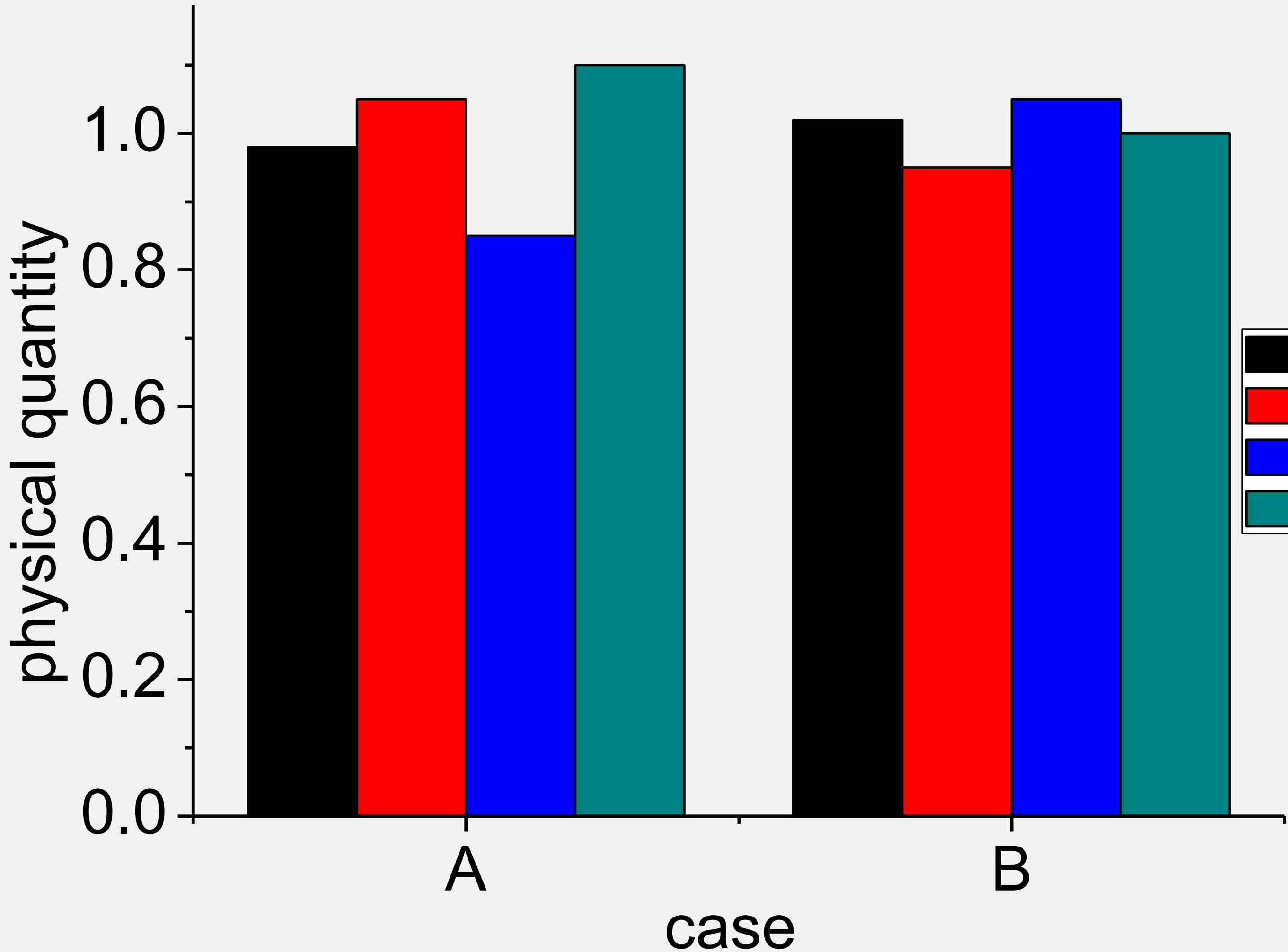
Jozef Stefan Institute,
Reactor Physics Division

- Experiment can serve as benchmark experiment, if performed with relatively low uncertainty
- Monte Carlo results can serve as benchmark for diffusion and/or transport codes

In a perfect world



Comparison



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Reactor Physics Division

Uncertaities

- Experiment
  - Measurement (measured physical quantity)
  - Material
  - Geometry
  - Temperature
  - other
- Calculation
  - Statistical
  - Nuclear data (cross section, emission spectra, Q values,…
  - other

Sensitivity studies

$$\sigma_i = \frac{dk}{dP_i}\sigma_{P_i}, \quad \frac{dk}{dP_i} \equiv \text{sensitivity coefficient}$$

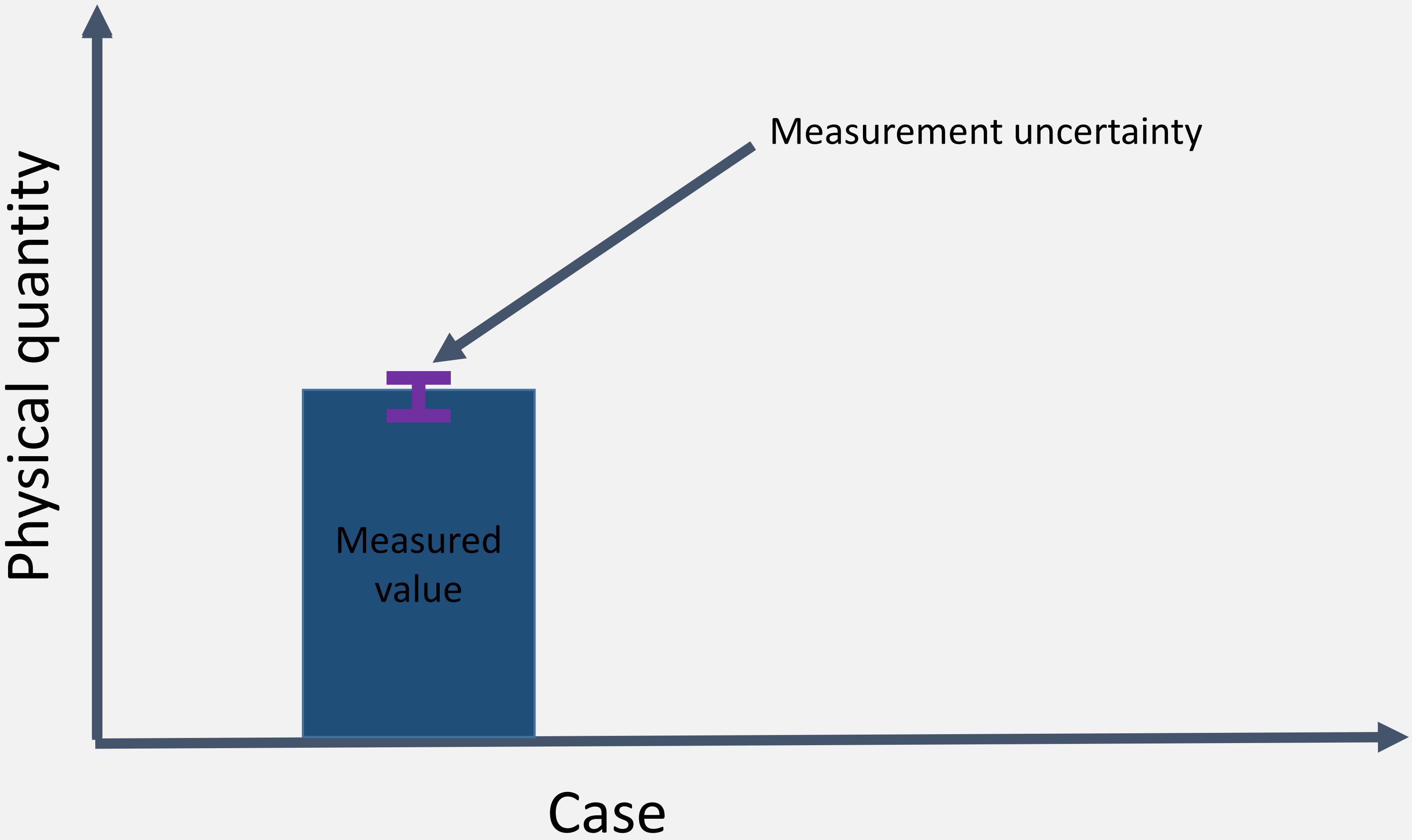
biases

- Mostly due to simplifications
  - Geometry
  - Materials
  - Computational methods
  - Other…
- Bias also has features uncertainty

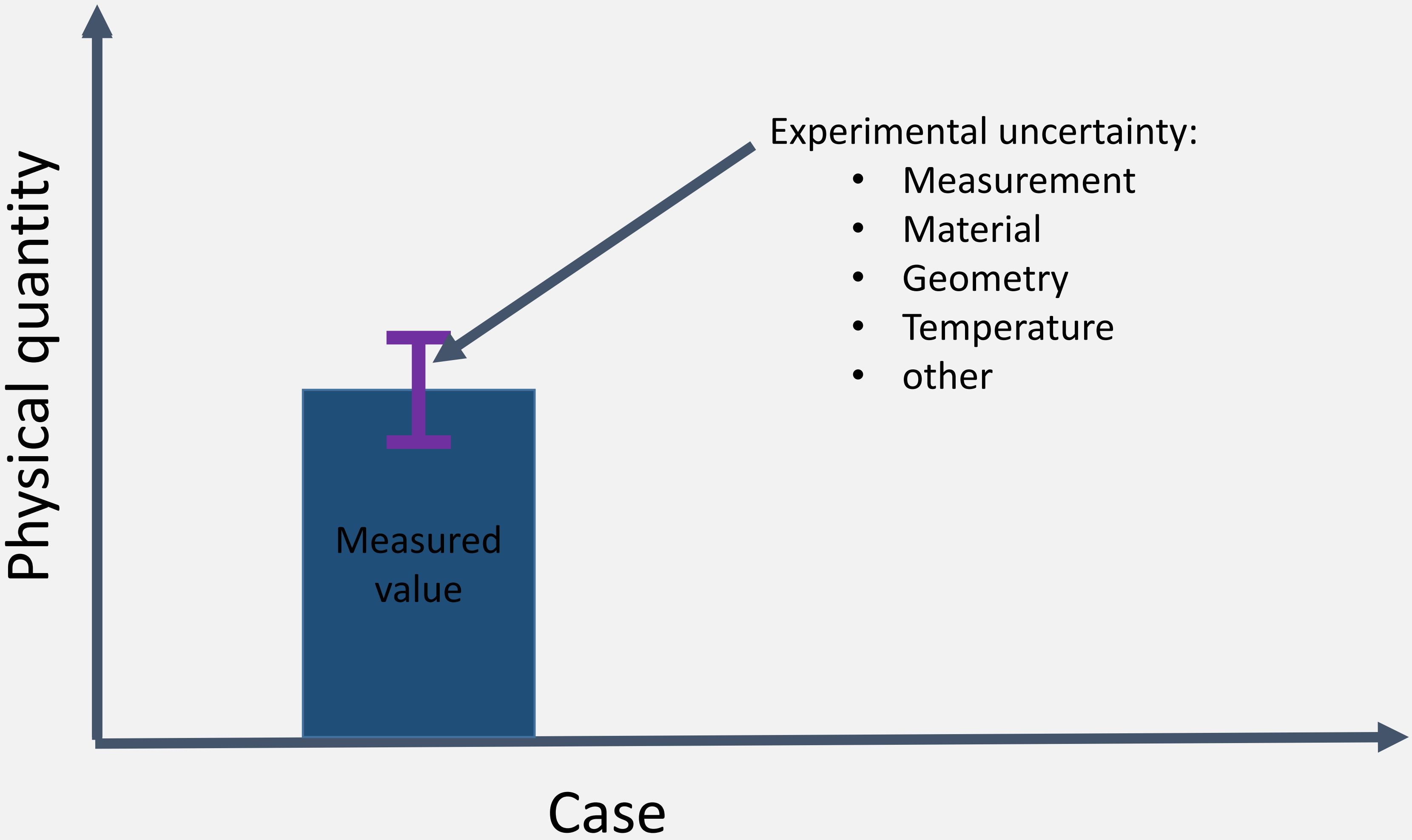
Benchmark model

- Model of the experiment suitable for computatonal modelling – can be simplified
- Benchmark model uncertainty
  - Experimental uncertainty + bias uncertainty
- Computational uncertainty
  - Statistical uncertainty + nuclear data uncertainty

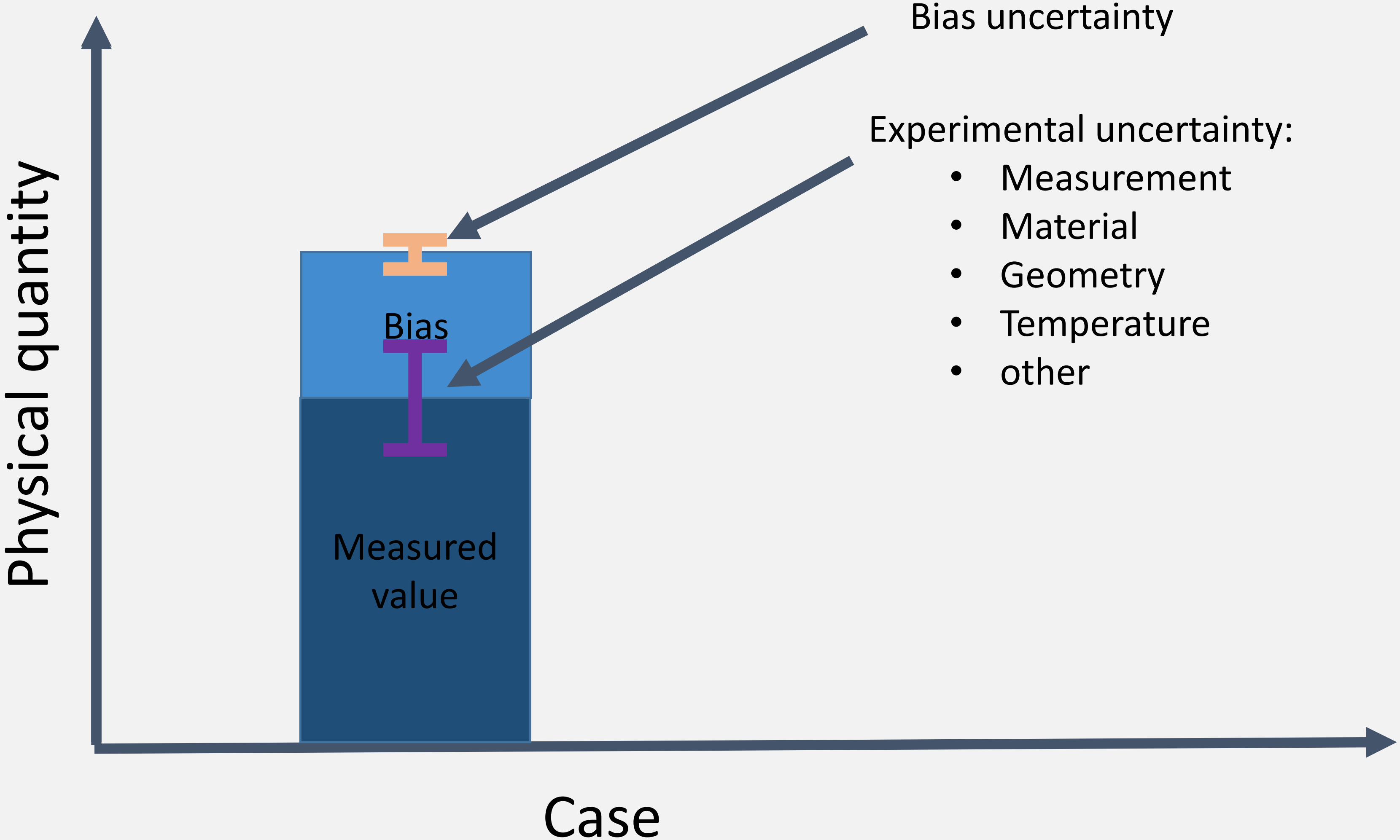
Uncertainties explained



Uncertainties explained



About Uncertainties

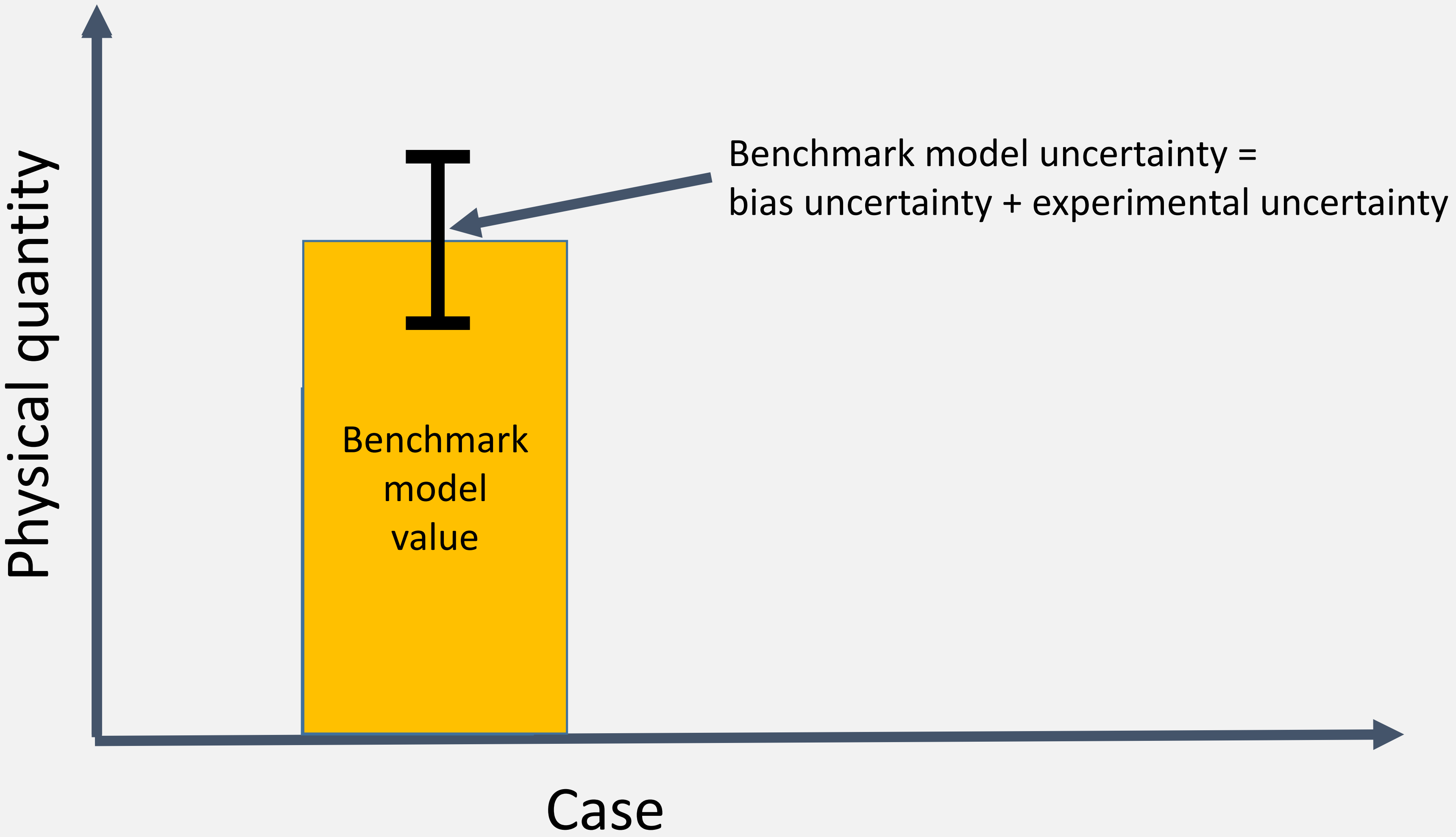


Bias uncertainty

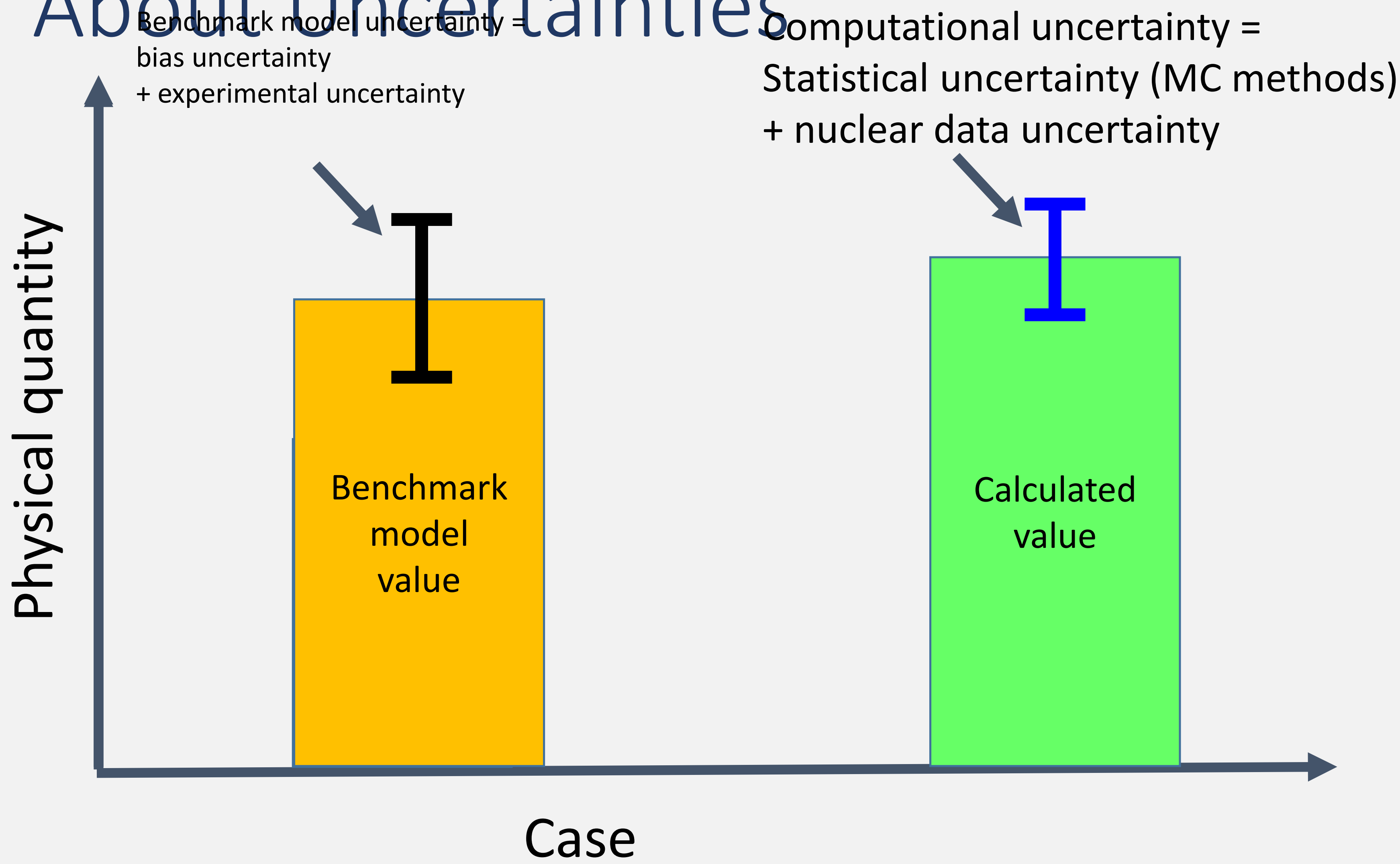
Experimental uncertainty:

- Measurement
- Material
- Geometry
- Temperature
- other

About Uncertainties



About Uncertainties



Data sources

- All relevant geometry and material data should be in principle contained in the Final Safety Analysis Report (FSAR) of the reactor. In practice, only part of these information is found there.
- It is also not very reliable and accurate since the, reactor description in SAR is often based on generic and not on “as built” data.
- The most reliable source of practical data is the design documentation of the reactor (plans, blueprints, drawings, fabrication specifications). It contains normally detailed data on geometry but only general data on material specifications.

Material data

- The material data are normally found in internal reports of the reactor manufacturer or in general literature
- Such data are, however, also mainly generic and normally approximately correspond to the particular case.
- The exception are the data about the enrichment and mass of uranium which are part of the safeguard documentation and are for this reason in details provided together with the fuel elements.
- The rest of the material data (e.g, material density, metallurgical composition in case of alloys, impurities important for neutrons, concentration of burnable poisons, ...) are normally not available for the particular reactor, especially if the reactor is old.